(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
7 April 2011 (07.04.2011)

PCT

(10) International Publication Number
WO 2011/039735 A2

(51) International Patent Classification:

A61K 31/53 (2006.01)	*G06F 19/00* (2011.01)
A61K 31/17 (2006.01)	*C07C 275/28* (2006.01)
A61K 31/426 (2006.01)	*C07C 275/30* (2006.01)
A61K 31/427 (2006.01)	*C07D 251/66* (2006.01)
A61K 31/4725 (2006.01)	*C07D 277/34* (2006.01)
A61P 35/00 (2006.01)	*C07D 277/38* (2006.01)
A61P 31/12 (2006.01)	*C07D 403/12* (2006.01)

(21) International Application Number:
PCT/IB2010/054475

(22) International Filing Date:
4 October 2010 (04.10.2010)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
61/248,030 2 October 2009 (02.10.2009) US

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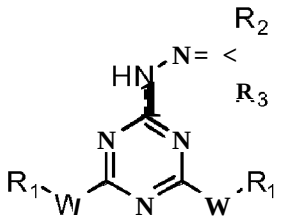
(81) Designated States *(unless otherwise indicated, for every kind of national protection available):* AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available):* ARIPO (BW, GH,

[Continued on next page]

(54) Title: COMPOUNDS WITH DDX3 INHIBITORY ACTIVITY AND USES THEREOF

(57) Abstract: The present invention relates to the medical use of the compound of formula 1, 2, 3 or 4:



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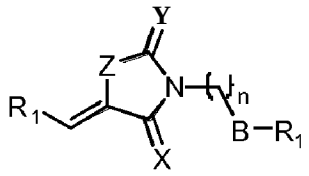

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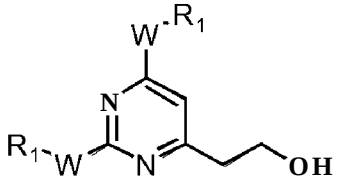

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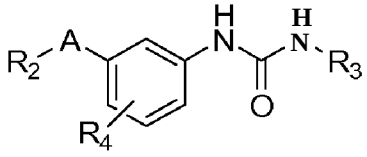

Formula 4

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GM, KE, LR, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— *without international search report and to be republished upon receipt of that report (Rule 48.2(g))*

COMPOUNDS WITH DDX3 INHIBITORY ACTIVITY AND USES THEREOF

Field of the invention

The present invention refers to compounds with cellular RNA helicase and /or ATPase DDX3 inhibitory activity and their therapeutic use, in particular for the treatment of viral and neoplastic diseases. The invention relates also to a method for identifying compounds endowed with binding capacities to the target sites on DDX3.

Background of the invention

DDX3 and HIV-1 infections

Cellular cofactors as potential novel targets for suppressing HIV-1 replication.

All compounds that are currently approved for the treatment of HIV infections target viral proteins: The enzymes reverse transcriptase (RT), protease (PR), integrase (IN) and, introduced more recently, the fusion peptide gp41 of the viral Env, which is essential for HIV entry. In considering how to design antiviral drugs, one could envision two different strategies. In fact, since viruses, including HIV, have evolved the capacity to exploit the cell's molecular machineries as essential components of their replicative cycle, agents designed to interrupt viral replication could, in principle, target with equal effectiveness either a viral or cellular polypeptide. These two strategies hold different implications. In the case of a unique viral function, such as retrotranscription or virion assembly, there is a lower risk of creating inhibitors with toxic effects on the host. However, the Achilles' heel of such an approach is viral resistance to the drugs. Unless a drug is incredibly potent (reducing the size of the replicating pool of virus rapidly), and therefore requires only a short duration of treatment (reducing the time for the resistant viruses to amplify), resistance to treatment will arise over time, as observed with HIV or HBV patients on therapy. The alternative approach, targeting a cellular factor that is required for viral replication should help to overcome the problem of viral resistance, but it has a major potential of causing greater toxicity to the host. Theoretically, a drug targeting a cellular factor could inhibit all viruses that are dependent on the same host factor. Thus, it has become a paradigm in antiviral research, that the understanding of the dynamic interplay of host cell and virus is essential to develop effective strategies for controlling viral infection. This holds true also for HIV. It has been shown that several cellular proteins are employed as essential co-factors by HIV. Established co-factors for HIV replication are the

chemokine receptors, CXCR4 and CCR5, that, in conjunction with CD4, are essential for viral entry into target cells. But also after entry, cellular proteins play essential roles within the viral replication cycle. Cellular binding partners exist for example for HIV-1 integrase such as integrase interactor 1 (Inil) which has amino acid similarity to the yeast transcriptional activator SNF5, a component of the multiprotein SWI/SNF complex (Kalpana et al., 1994), and HMGA1, a non-histone chromosomal protein important for transcriptional control and chromosomal architecture (Farnet and Bushman, 1997). The Debyser group has recently identified Lens Epithelium Derived Growth Factor (LEDGF) as a novel binding partner of HIV-1 integrase (Cherepanov et al, 2003), using Fluorescence Cross Correlation Spectroscopy as an innovative technology to study protein-protein interactions in the living cell (Maertens et al., 2005). Besides integration, other steps of the replicative cycle of HIV-1 require the essential contribution of specific cellular proteins, including viral transcription (cellular Cyclin T1 (Wei et al., 1998)) and viral assembly and egress (e.g. TSG101, a member of the cellular ESCRT machinery (von Schwedler et al., 2003)). From another perspective, the critical role of cellular co-factors gains strong support from the finding that HIV-1 is unable to replicate in non-human cells, including cells from non-human primates, mice, and rats (Cohen, 2001). Apparently, HIV-1 replication is subject to potent restrictions in these species. Over the years, important advances have been made in elucidating the molecular basis of such blocks to HIV-1 replication, with a particular emphasis on rodent cells. In fact, the critical role of several cellular co-factors for HIV-1 infection, including the CXCR4 co-receptor and the transcription enhancing factor Cyclin Tl, which is a component of the pTEFb transcription factor complex (Wei et al, 1998), was first identified in mouse cells. Expression of the human protein, but not of the mouse ortholog, allowed the HIV replication cycle to progress. Remarkably, a single amino acid difference between mouse and human Cyclin T1 appears to determine its ability to interact with the viral Tat protein. Subsequent inhibition or knock-down studies in human cells confirmed the pivotal role of CXCR4 and Cyclin T1 for HIV-1 replication. Thus, the characterization of intrinsic restrictions in the HIV-1 replication cycle in rodent cells is a powerful approach for the identification of essential cellular co-factors and potential drug targets in human cells. Furthermore, pinpointing such species-specific restrictions provides the basis to overcome these blocks and advance the development of a fully-permissive transgenic small animal model of HIV-1 infection (Cohen, 2001). Here, the Keppler group previously demonstrated that immuno-

competent rats, that transgenically express the human CD4/CCR5 receptor complex, support a robust cellular infection and transient, low-level viremia (Keppler et al, 2005; Keppler et al., 2002; Keppler et al, 2001). In particular primary macrophages from transgenic rats supported the full HIV-1 replication cycle and secreted infectious virions.

The essential Rev-dependent HIV RNA nuclear export pathway and the role of the RNA helicase DDX3.

The nuclear export of viral RNAs is a crucial step in HIV-1 replication, since the appropriate expression of viral genes paves the way to all the following steps like encapsidation, virion assembly and budding. Any drug targeting this step will act at an earlier level than protease inhibitors, shutting down viral proliferation at a step where no structural viral proteins (Gag-Pol, Env) or even full length genomic RNA have yet been produced in the infected cells. Due to its outmost importance, it is of no surprise that the export of partially spliced or unspliced viral transcripts is one of the most complex and tightly regulated steps of the entire HIV-1 life cycle. It has to be stressed that normal, uninfected cells have evolved strict quality control pathways to avoid the nuclear export of partially spliced transcripts, in order to ensure that no aberrant proteins will be produced upon translation by ribosomes (Cullen, 2003). Thus, in order to allow nuclear export of its own unprocessed or partially processed transcripts, HIV-1 has to completely subvert and take control of these cellular machineries, and this is why at this particular step of the viral life cycle, functional interactions between viral and cellular proteins do likely play a pivotal role.

The Rev/RRE-dependent HIV RNA export pathway.

All nucleo-cytoplasmic transport processes take place through the nuclear pore complex (NPC), a large dynamic multi-protein assembly that acts as the passageway for transport (Pante, 2004). This active transport can also occur against a concentration gradient, and is mediated by soluble transport factors, that in turn shuttle between the nucleus and the cytoplasm. Importantly, even molecules that are theoretically small enough for passive diffusion (e.g., HIV-1 Rev) are actively and selectively transported, since regulated transport appears to be more efficient and more amendable for specific regulation (Pemberton and Paschal, 2005).

HIV-1 has a total of nine genes that are expressed by alternative splicing of a single, initial proviral transcript that also forms the RNA genome. Importantly, HIV-1 replication requires the nuclear export and translation of unspliced, singly-spliced and multiply-spliced derivatives of this initial transcript. Fully spliced mRNAs encode the viral regulatory proteins Tat, Rev and Nef, whereas incompletely spliced HIV-1 mRNAs primarily encode viral auxiliary (Vif, Vpr, Vpu) and structural proteins. The HIV-1 Rev is a sequence-specific nuclear mRNA-export factor. In the absence of Rev function, the incompletely spliced HIV-1 mRNAs that encode the viral structural proteins are retained in the cell nucleus, whereas nuclear export of fully-spliced HIV-1 mRNAs, including the mRNA encoding Rev itself, is independent of Rev function. Nuclear export of unspliced HIV-1 mRNAs also requires a structured cis-acting RNA sequence, called the Rev response element (RRE), which is specifically bound by Rev. The nuclear retention of the incompletely spliced viral mRNAs in the absence of Rev results from the fact that splice sites present in the retained introns are recognized by cellular mRNA processing factors, termed splicing commitment factors, that normally prevent cellular pre-mRNAs (i.e. incompletely spliced cellular mRNAs) from exiting the nucleus. (Cullen, 2003). The HIV-1 Rev protein has two distinct functional domains, an N-terminal sequence required for RRE binding and Rev multimerization and a 10-amino-acid leucine-rich domain near the C-terminus that serves as the Rev nuclear export signal (NES). This signal mediates the nuclear export of the Rev/RNA complex, through interaction with the cellular export receptor Crml and proposed additional cellular cofactors (Yedavalli et al., 2004).

The Crml-dependent cellular RNA export pathway.

Crml is a member of the karyopherin-beta family of nucleocytoplasmic-transport factors. Karyopherin-beta members associate with karyopherin-alpha in the cytoplasm, forming a heterodimeric complex with proteins containing a nuclear localisation signal (NLS). Then, karyopherin -beta interacts with the nuclear pore complex (NPC), facilitating the import of the karyopherin -alpha/NLS -protein complex. Recently, however, members of the karyopherin -beta family have been identified which regulate nuclear export, rather than import, pathways. One of such proteins is Crml, which shares homology with karyopherin betal, beta2, beta3 and beta4. Human Crml is localized both at the NPC and in the nucleoplasm and seems to shuttle between the nucleus and cytoplasm. It is now clear that Crml is the crucial nuclear export factor for two classes of cellular RNAs, that is, U-rich

small nuclear RNAs and ribosomal RNAs. Crml binds its cargo in the nucleus in the presence of the GTP-bound form of the Ran GTPase. After nuclear export, hydrolysis of the bound GTP to GDP causes a conformational shift that induces cytoplasmic cargo release, thus providing the directionality of this export pathway. Crml also interacts with components of the NPC, the portal used for all nucleocytoplasmic transport, and this interaction is essential for Crml -mediated nuclear RNA export.

The DDX3 family of cellular RNA helicases.

Recently, the DEAD-box RNA helicase DDX3 was identified as an essential cofactor for Rev/RRE-mediated HIV RNA-export (Yedavalli et al, 2004). RNA helicases from the DEAD-box family are found in almost all organisms and have important roles in RNA metabolism. They are associated with many processes ranging from RNA synthesis to RNA degradation. DEAD-box proteins use the energy from ATP hydrolysis to rearrange inter- or intra-molecular RNA structures or dissociate RNA-protein complexes. Human DEAD-box family includes 36 members. The majority of DEAD-box family members have demonstrated functions in ribosome biogenesis and translation initiation. In addition to a function in RNA metabolism, two other functional features appear to be present in this gene family. The first feature is dysregulation in cancer, which occurs in the form of involvement in recurrent chromosomal translocations *(DDX6, DDX10)* or overexpression *(DDX1, DDX6, DDX4).* The second feature is the involvement of *DDX* members in tissue-organ differentiation *(DDX4* in germ cell development, *DDX5* in organ differentiation, *DDX25* in spermatogenesis, and *DDX41* in visual system development). Therefore, putative RNA helicases may have a function in differentiation, possibly by their effect on the expression of critical differentiation genes.

The human cellular RNA helicase DDX3/HIV-1 Rev axis.

DDX3 expression was found to be induced in HIV-1 infected cells by the viral transcriptional activator Tat, but it apparently plays no role in HIV-1 transcription. Instead, DDX3 was shown to be an RNA-dependent ATPase/helicase which functions in the Rev-RRE/CRMl pathway for the export of unspliced/partially spliced HIV-1 transcripts. DDX3 is a nucleo-cytoplasmic shuttling protein that binds Crml and associates to the cytoplasmic side of nuclear pores. Its enzymatic activity, as well as its physical interaction with Crml is

necessary for Rev/RRE mediated nuclear export of viral RNAs. However, the molecular details of its role(s) in this pathway are yet to be elucidated.

DDX3 and HBV/HCV infections

A significant downregulation of DDX3 expression is found in hepatocellular carcinoma (HCCs) from hepatitis B virus (HBV)-positive patients, but not from HCV-positive ones, compared to the corresponding nontumor tissues. The expression of DDX3 is differentially regulated by the gender and, moreover, there is a tendency that the downregulation of DDX3 expression in HCCs is more frequent in males than in females. Genetic knockdown of DDX3 with small interfering RNAs (siRNA) in a nontransformed mouse fibroblast cell line, NIH-3T3, results in a premature entry to S phase and an enhancement of cell growth. This enhanced cell cycle progression is linked to the upregulation of cyclin D1 and the downregulation of p21(WAFl) in the DDX3 knockdown cells. In addition, constitutive reduction of DDX3 expression increases the resistance of NIH-3T3 cells to serum depletion-induced apoptosis and enhances the ras-induced anchorage-independent growth, indicating the involvement of DDX3 in cell growth control. These suggest that the deregulation of DDX3, a DEAD box RNA helicase with cell growth-regulatory functions, is involved in HBV- and HCV-associated pathogenesis. Owsianka and Patel (1999) have shown that DDX3 interact specifically with hepatitis C virus (HCV) core protein and thus resulted in a change of its intracellular location. Huang *et al.* (2004) have demonstrated that the mRNA expression of DDX3 is up-regulated in hepatocellular carcinoma (HCC). Since many lines of evidence indicate that HCV core protein is the oncogenic agent that activates the neoplastic transformation pathways in HCC, the overexpression of DDX3 in HCC tissue could play a role in the downstream transformation pathway or in synergy to the transformation capability of HCV core protein in HCC.

DDX3 and cancers

Chao *et al.* (2006) showed that the subcellular localization of DDX3 is alterated in cutaneous squamous cell carcinoma (SCC).

In 2008 Botlagunta *et al.* (2008) using immortalized breast cell lines and breast cancer cells, showed that DDX3 expression correlates with an aggressive tumoral phenotype. The human breast cell line, MCF 10A, was characterized for the gene expression pattern. Of the differential genes expressed, it was found consistent activation of DDX3, a member of

the DEAD box RNA helicase family. Overexpression of DDX3 in MCF 10A cells induced an epithelial-mesenchymal-like transformation, exhibited increased motility and invasive properties, and formed colonies in soft-agar assays. Besides the altered phenotype, MCF 10A-DDX3 cells repressed E-cadherin expression as demonstrated by both immunoblots and by E-cadherin promoter-reporter assays. In addition, an in vivo association of DDX3 and the E-cadherin promoter was demonstrated by chromatin immunoprecipitation assays. Collectively, these results demonstrate that the activation of DDX3 by BPDE, can promote growth, proliferation and neoplastic transformation of breast epithelial cells.lt is possible that the regulatory mechanisms of DDX3 in various cell types are different depending upon the presence of appropriate cofactor and/or signaling pathways

As indicated above, current pharmacological therapies against HIV-1 infections are based on multiple drug combinations. Most used and cornerstone drugs act upon viral enzymes: reverse transcriptase (RT), protease (PR), integrase (IN). In addition, one class of drugs inhibits HIV entry in cells by competing for the recepetor/coreceptor usage. While drugs directed against RT and PR are widely used, their efficacy is hampered by mutations in the target enzymes, leading invariably to drug resistance and chemotherapy failure.

The protein DDX3 has been shown to 1) be an essential cofactor for the replication of the HIV-1 and HCV viruses; 2) be involved in the proliferation of cancer cells. The DDX3-inhibitors are therefore considered as potential agents not only in the treatment of HIV-1 infections, but also for other viruses such as HCV, as well as in the treatment of various kinds of cancer, such as hepatocellular carcinoma.

The combination of DDX3-inhibitors to the existing antiviral and anticancer therapy would also improve the outcome of the treatment.

No inhibitors of DEAD-box RNA helicases DDX3 have been described so-far. A compound has been recently published as a DDX3 inhibitor (Yedavalli, V. S. R. K. et al. *J. Med. Chem.* **2008,** *51,* 5043-5051). However, direct inhibition of RNA helicases has not been proven.

Maga et al. *(J. Med. Chem.* **2008,** *51,* 6635-6638) disclose a receptor-based Pharmacophore Models of the ATP-binding site to be used for the identification of DDX3 inhibitors. The three dimensional arrangements of the functional groups of an inhibitor described by the Pharmacophoric Models (essential for the effective binding to DDX3) has been used for a three-dimensional (3D) database search.

The present invention describes compounds with cellular DDX3 inhibitory activity and their use in the treatment of viral and neoplastic diseases. A method for the identification of such inhibitors, based on an homology model of the closed conformation of DDX3 to locate the RNA-binding site and Virtual Docking protocol is disclosed. The synthesis of the compounds is also provided.

The invention illustrate a novel approach to treat HIV/AIDS, namely targeting a cellular enzyme (the DEAD-box RNA helicases DDX3) which has been recognized as a co-factor for HIV replication, thus rendering the infected cell an unfavorable environment for viral replication. The advantage of such approach is ideally represented by the possibility to overcome the drug resistance problem connected to common anti-HIV drugs, since cellular enzymes do not have the high mutation rates typical of viral enzymes.

Summary of the invention

The present invention describes compounds able to suppress the enzymatic functions of the cellular protein DDX3 (Dead-box polypeptide 3; Ref. Seq. NP_001347), namely: ATP hydrolysis (ATPase) and/or DNA/RNA unwinding (helicase).

The compounds presented in this invention (Formula 1-4) surprisingly showed:

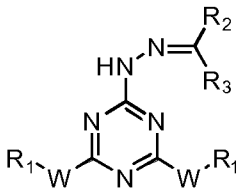
1) the ability to selectively suppress the enzymatic activity of DDX3 in vitro;

2) the ability to suppress HIV-1 replication in infected cells;

3) the ability to suppress proliferation of tumor cell lines.

These experimental findings make the new compounds useful as both antiviral and anticancer therapy.

It is therefore an object of the invention a compound of formula 1, 2, 3 or 4 for use as a treatment of a pathology modulated by DDX3 activity and/or expression:



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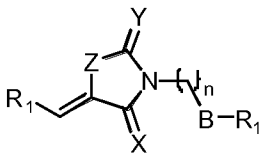

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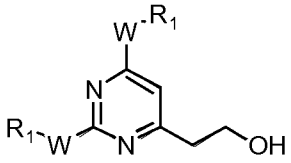

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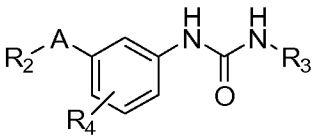


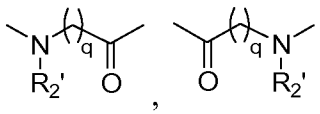
Formula 4

wherein:

Z represents CH_2 or S;

X and Y represent independently O or S;

n is comprised between 0 and 4;

B is absent or represents  q is comprised between 0 and 2 and R_2' represents H, $-(CH_2)_{W'}-OH$, $-(CH_2)_{w'}-NH_2$, w' is an integer from 1 to 3; B is also C=0;

Ri, R_2, R_3 are each independently selected from the group of: H, a linear or branched alkyl group comprising 1 to 6 carbon atoms, unsubstituted or substituted phenyl radical, an unsubstituted or substituted phenylalkenyl radical, an unsubstituted or substituted phenyalkynyl radical, an unsubstituted or substituted biphenylalkyl radical, an unsubstituted or substituted heterocyclic radical, an unsubstituted or substituted polycyclic radical, an unsubstituted or substituted alicyclic radical or a radical of the formula $(Ria-)_m(L-)_pRib-$, wherein Ria and Rib may be the same or different and represent an unsubstituted or substituted heterocyclic radical or an unsubstituted or substituted phenyl radical, Ria also represents an unsubstitutetd or substituted polycyclic radical and L represents a divalent linking moiety selected from the group consisting of a valence bond, $-(CH_2)q-$, -HC=CH-, -C≡C-, -C(=0)-, -0-, -S-, -S(=0)-, $-S(=0)_2-$, -NHCONH- or NR_1C, RiC being hydrogen or alkyl, m and p are each independently 0 or 1, and q is an integer from 1 to 3;

R_2 and R_3 together optionally form a cycloalkyl, cycloalkenyl, non-aromatic heterocyclic, or fused or polycyclic ring, 2-oxindole wherein said cycloalkyl, cycloalkenyl, non-aromatic heterocyclic and fused or polycyclic ring are optionally substituted with one or more substituents selected from the groups above described. Examples of suitable fused or polycyclic ring are substituted or unsubstituted 2-oxindoles; substituted or unsubstituted lH-indene-l,3-diones

wherein the heterocyclic radical is selected from the group consisting of morpholine, thiomorpholine, piperidine, piperazine, pyrrolidine, furan, thiophene, oxazole, oxadiazole, isoxazole, pyridine, 1,3-oxathiolane, thiazole, isothiazole, thiadiazole, imidazole, pyrrole, tetrazole or triazine;

wherein the polycyclic radical is selected from the group consisting benzofuran, isobenzofuran, benzothiophene, isobenzothiophene, benzoxazole, indole, 2-isoindole, 2-oxindole, 2-methylindole, benzopyrazole, quinoline, isoquinoline, tetrahydroquinoline, 1,3-benzodioxole, 1,2-benzodiazine, 1,3-benzodiazine, 1,2,3-benzotriazole, benzothiazole, benzimidazole, 1,2,3-benzotriazine, 1,2,4-benzotriazine, naphtalene, antracene or fluorene;

wherein the alicyclic radical preferably comprises 5 to 8 carbon atoms. Examples of suitable cycloalkyls are cyclopentyl, cyclohexyl, methylcyclohexyl and norbornyl.

wherein the heterocyclic radical substituents, the polycyclic radical substituents and the alicyclic radical substituents being at least one selected from the group consisting of straight or branched chain, saturated or unsaturated aliphatic group having 1-6 carbon atoms, halogen, perhaloalkyl, monohaloalkyl, dihaloalkyl, alkoxy, acyl, acyloxy, acyloxyalkyl, phenylalkoxy, hydroxy, hydroxyalkyl, thio, alkylthio, nitro, carboxy, carbalkoxy;

wherein the phenyl radical substituents, the phenylalkenyl radical substituents, the phenylalkynyl radical substituents or the biphenylalkyl radical substituents are selected from the group consisting of a straight or branched chain, saturated or unsaturated aliphatic group having 1-6 carbon atoms, halogen, nitro, carboxy, carboxy alkyl, alkoxy, hydroxy, hydroxyalkyl, perhaloalkoxy, acyl, acyloxy, acyloxyalkyl, cyano, carbalkoxy, thio, alkythio, alkylsulfmyl, alkylsulfonyl, amino, alkylamino, dialkylamino, aminoalkyl, alkylaminoalkyl, dialkylaminoalkyl, sulfonamido, carboxamido, alkanoylamino;

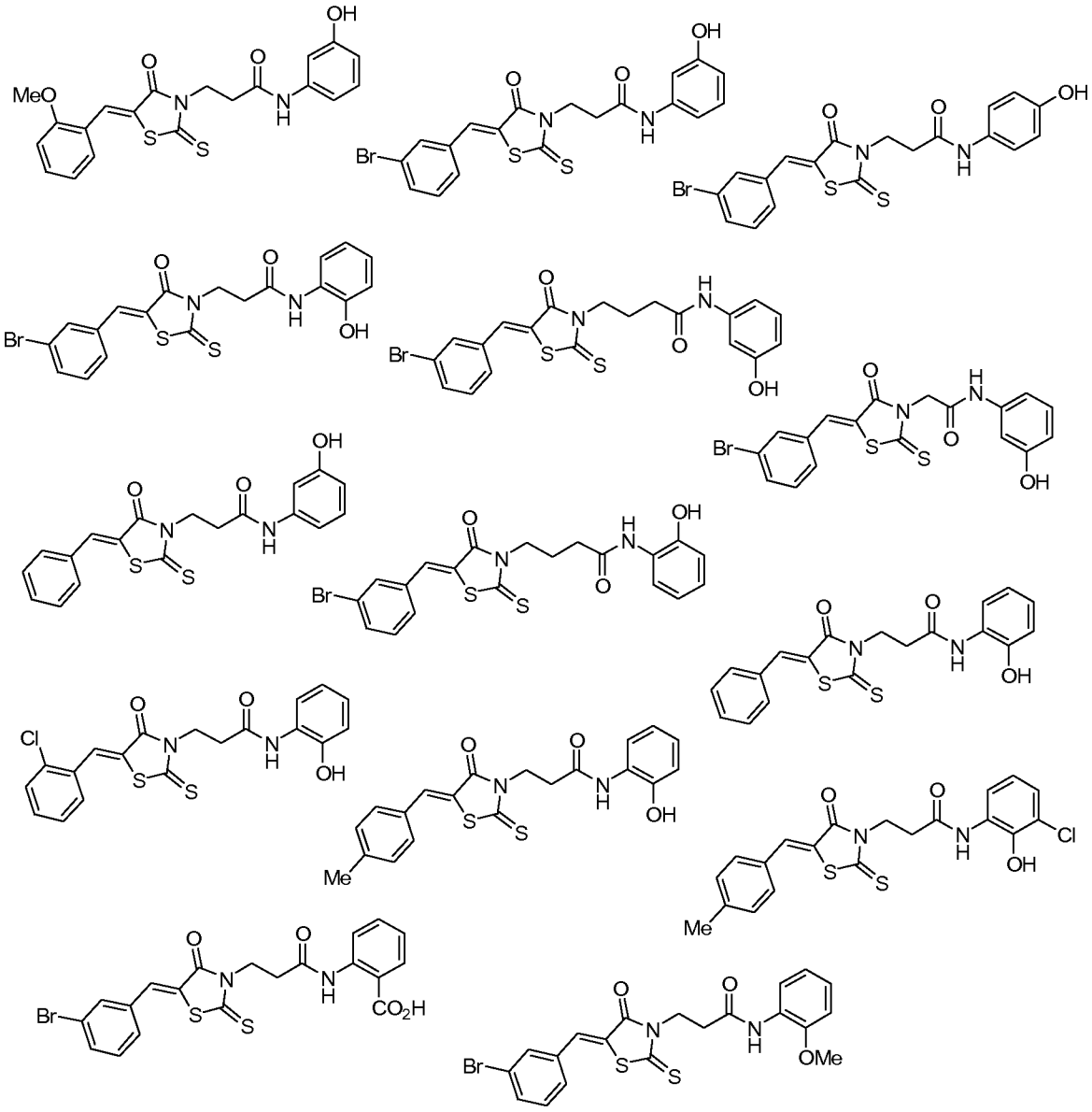
W is absent or represents independently O, S, NH, $NHCH_2$ or N-R_5 wherein R_5 is a linear or branched alkyl group comprising 1 to 6 carbon atoms;

A is absent or represents CONH, NHCO, NHCONH;

R_4 represents H, unsubstituted or substituted alkyl from 1 to 6 carbon atoms, unsubstituted or substituted alkenyl, unsubstituted or substituted alkynyl, halogen, haloalkyl, COOH,

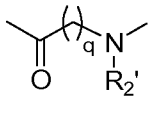
OCH_3, $N0_2$, NH_2, CN, OZ' or SZ' where Z' is H, or unsubstituted or substituted alkyl from 1 to 6 carbon atoms;

with the provisio that the compounds indicated below are not comprised



Preferably, the compound has formula 1 or 3 wherein W is absent or independently selected from NH, $NHCH_2$ or N-R5 wherein R_5 ethyl; Ri is independently selected from the group of ethyl, heterocyclic radical, unsubstituted or substituted phenyl radical and polycyclic radical; R_2 is selected from the group of unsubstituted or substituted phenyl radical, heterocyclic radical or polycyclic radical when R_3 = H or Me; alternatively, R_2 and R_3 together form a 2-oxindole.

Still preferably, the compound is the compound l id, 14f, 14g, 15h, 15k, 38, FE56, FE56M, FE56F, FE56N, FE56AN or 22.

In a preferred embodiment, the compound has formula 2 wherein Z = S; Y = S; X = 0 ; n = 2; B =  or C=0; q = 0; R_2' = H; Ri is independently selected from the group of substituted phenyl radical or polycyclic radical

Still preferably, the compound is the compound 35b, 35c, 35f, FE-70, FE-77, FE-69, FE-74.

Preferably, the compound has formula 4 wherein R_2, R_3 are independently selected from the group of H, unsubstituted or substituted phenyl radical; R_4 = H, unsubstituted or substituted alkyl from 1 to 6 carbon atoms, COOH, OCH_3, $N0_2$, NH_2; A is absent or represents CONH, NHCO, NHCONH.

Still preferably, the compound is the compound EI-01, EI-01A, EI-01B, 25, 26, 27, 29, 30, 31.

Preferably the compound is an inhibitor of the human DEAD-box RNA helicases DDX3.

Still preferably the compound is an inhibitor of ATPase and/or helicase of the human DEAD-box RNA helicases DDX3.

In a preferred embodiment the pathology modulated by DDX3 activity and/or expression is an infection or a hyperproliferative disease. Preferably, the infection is a viral infection. Still preferably, the viral infection is caused by HIV, HBV, HCV or poxviruses. More preferably it is caused by HIV-1.

In a preferred embodiment the hyperproliferative disease is a tumor. Preferably, the tumour is selected from the group of: hepatocellular carcinoma, cervical cancer, breast cancer, lymphomas, leukemias.

It is a further object of the invention a pharmaceutical composition comprising the compound as defined above, or a pharmaceutically acceptable salt, solvate, or hydrate thereof and pharmaceutically acceptable excipients for use as a treatment of a pathology modulated by DDX3 activity and/or expression.

In the present invention a pathology modulated by DDX3 activity and/or expression is defined as a pathology that can be induced, trigerred or enhanced by DDX3 protein. The activity of DDX3 can be measured by techniques known in the art for instance by measuring the enzymatic activity of the protein (ATPase or helicase activity). The expression of DDX3 is also measured by commonly used methods in the art. The compounds of the present invention are particularly suitable for the treatment of patient

that are resistant to at least one currently used treatment for HIV infection. For instance, patient resistant to RT inhibitors, PR inhibitors and/or IN inhibitors.

In the present invention the compounds as defined above and suitable excipients and/or diluents may be administered in combination with pharmaceutical compositions of approved drugs for the treatment of the HIV-1 infections as part of highly active antiretroviral therapy (HAART).

The pharmaceutical composition of the invention may comprise a combination of at least two of the compounds of the invention or a pharmaceutically acceptable salt thereof, and suitable excipients and/or diluents and may be also administered in combination with pharmaceutical compositions of approved drugs for the treatment of the HCV infections as part of combinatorial multidrug anti-HCV therapy.

The pharmaceutical composition of the invention may comprise a combination of at least two of the compounds of the invention or a pharmaceutically acceptable salt thereof, and suitable excipients and/or diluents and may be also administered in combination with pharmaceutical compositions of approved drugs for the treatment of cancers as part of combinatorial multidrug cancer therpay.

Preferably the pharmaceutical composition comprising at least one or two of the compounds of the invention together with at least one approved compound for the treatment of HIV-1 infections are in the same formulation or a pharmaceutically acceptable salt thereof, and suitable excipients and/or diluents to be administered as such.

In the present invention the compounds of the invention or their salts may be administered as pure or as pharmaceutical formulations, i.e. suitable for parenteral, oral, or rectal administrations. Each of said formulations may contain excipients and/or fillers and/or additives and/or binders, coatings and/or suspending agents and/or emulsifying agents, preserving and/or control release agents, suitable for the selected pharmaceutical form.

It is a further object of the invention a method for inhibiting the human DEAD-box RNA helicases DDX3 comprising contacting the compound of the invention or the composition as defined above with human DDX3, thereby inhibiting the activity of DDX3.

It is a further object of the invention a method for treating a viral and/or a hyperproliferative disease in a cell, comprising contacting the cell with the compound or the composition of the invention.

It is a further object of the invention a process for the preparation of the compound as defined above.

It is a further object of the invention a method for identifying a compound endowed with helicase inhibitory activity against the human DEAD-box RNA helicases DDX3 comprising using at least a portion of the homology model (namely the RNA binding site) of the close conformation of DDX3 as defined in Appendix I and Fig. 3.

Preferably, the method comprises:

(a) Providing a homology model of the close conformation of DDX3 as defined in Appendix I;

(b) providing a candidate compound;

(c) evaluating the level of binding of the candidate compound to the RNA-binding site of the human DEAD-box RNA helicases DDX3, wherein if a sufficient level of binding is found, then the compound is identified.

Preferably the candidate compound is selected from a library of compounds, selected from a from a database, is provided computationally, is designed de novo or is designed from a known DDX3 inhibitor.

Still preferably the sufficient level of binding is indicated by a calculated binding energy defined by a Chemscore value of at least 25.

It is a further object of the invention a compound identified by the method as described above.

Preferably the compound has the formula 4 as defined above.

It is a further object of the invention a composition comprising the compound identified by the method as described above or a pharmaceutically acceptable salt, solvate, or hydrate thereof and pharmaceutically acceptable excipients for use as a treatment of a pathology modulated by DDX3 activity and/or expression.

It is a further object of the invention a computer for producing a three-dimensional representation of the close conformation of DDX3 wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of the close conformation of DDX3 of Appendix 1;

(b) a working memory for storing instructions for processing said computer- readable data;

(c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three- dimensional representation.

It is a further object of the invention a machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structure co-ordinates of the close conformation of DDX3 of Appendix 1.

It is a further object of the invention the use of the computer or the machine readable data storage medium as defined above to predict the structure and/or function of potential modulators of DDX3.

The foregoing only summarizes certain aspects of the invention and is not intended to be limiting in nature. These and other aspects of the invention will be further elucidated in the following description and examples. The descriptions in the present invention are provided only as examples and should not be understood to be limiting on the claims. Based on the description, a person of ordinary skill in the art could make modifications and changes to the preferred embodiments, which does not depart from the scope of the present invention.

The invention will be now illustrated by means of non limiting examples referring to the following figures

Figure 1. A) Antiviral activity (expressed as % of viral load with respect to the control) of compounds FE56 and FE66 at 0.3 μM and 3 μM doses against single round HIV-1 replication in HeLaCD4+ cells infected with a wild type HIV-1 strain. Measurements were performed at 72 h post infection. B) Antiviral activity of compounds FE15 and FE66 on HIV-1 replication in phytohemagglutinin-stimulated peripheral blood mononuclear cells (PBMCs) transfected with HeLa $CD4^+$-cell culture supernatants containing wild type HIV. Compounds were tested at 50 μM (FE15) and 5 μM (FE66). The HIV-1 RNA was quantified in the cell culture supernatant after 3, and 5 days of incubation. Results are expressed as HIV RNA copies/ml. Control (white bars).

Figure 2. Antiviral activity of DDX3 inhibitors. A) Comparison of the antiviral activity (expressed as % of viral RNA with respect to the control) on infected PBMCs of a fixed dose of selected inhibitors. Measurements were performed at 72 h post infection. Values are the means of three independent replicates. Error bars are ±SD. White bars: control without drugs; dark grey bar: positive control with AZT (0.01 μM); black bar: first generation inhibitor **FE15** (50 μM); light grey bars: second generation DDX3 inhibitors **FE66, lid** and **38** (3 μM). B) Dose-response curves for the inhibiton of HIV-1 replication

(expressed as % of viral RNA with respect to the control) in infected PBMCs by **FE15** (circles) and **38** (triangles). Measurements were performed at 72 h post infection. Values are the means of three independent replicates. Error bars are ±SD.

Figure 3. Schematic representation of in silico DDX3-closed model preparation.

Figure 4. Schematic representation of in silico screening protocol (virtual docking) for the discovery of DDX3 inhibitors targeting the ATP- and/or the RNA-binding site.

Detailed description of the invention

MATERIAL AND METHODS

Synthesis

General. All commercially available chemicals were used as purchased. C¾CN was dried over calcium hydride, *t*BuOH was dried over Mg/I_2, CH_2C1_2 was dried over sodium hydride and THF and dioxane were dried over Na/benzophenone prior to use while DMF was bought already anhydrous. Anhydrous reactions were run under a positive pressure of dry N_2 or argon. IR spectra were recorded on a Perkin-Elmer BX FTIR system, using KBr pellets. TLC was carried out using Merck TLC plates silica gel 60 F254. Chromatographic purifications were performed on columns packed with Merk 60 silica gel, 23-400 mesh, for flash technique. 1H-NMR and ^{13}C-NMR spectra were recorded at 400 MHz on a Brucker Avance DPX400, at 300 MHz on a Varian VXR-300 and at 200 MHz on a Bruker AC200F spectrometer. Chemical shifts are reported relative to tetramethylsilane at 0.00 ppm. Elemental analyses (C, H, N) were performed in-house using a Perkin-Elmer Elemental Analyzer 240C. Melting points were taken using a Gallenkamp melting point apparatus and are uncorrected. Mass spectra (MS) data were obtained using an Agilent 1100 LC/MSD VL system (G1946C) with a 0.4 mL/min flow rate using a binary solvent system of 95:5 methyl alcohol/ water. UV detection was monitored at 254 nm. Mass spectra were acquired in positive and negative mode scanning over the mass range.

Microwave Irradiation Experiments. Microwave irradiation experiments were conducted using a CEM Discover Synthesis Unit (CEM Corp., Matthews, NC). The machine consists of a continuous focused microwave power delivery system with operator-selectable power output from 0 to 300 W. The temperature of the contents of the vessels was monitored using a calibrate infrared temperature control mounted under the reaction vessel. All the experiments were performed using a stirring option whereby the contents of

the vessel are stirred by means of rotating magnetic plate located below the floor of the microwave cavity and a Teflon-coated magnetic stir bar in the vessel.

Biology

Enzymatic assays

Human DDX3 ATPase activity assay

ATPase activity was tested with a luciferase-based luminescence assay (Easylite-Kinase, Perkin Elmer) on 96 wells microtiter plates. Briefly, recombinant purified human DDX3 (50-100 ng) was incubated in a 15 μL total reaction volume with reaction buffer (25 mM TrisHCl pH 7.5, 5 mM $MgCl_2$), in the presence of increasing amounts of ATP and/or different combinations of ATP and the inhibitor to be tested. Reference curves in the absence of inhibitor (giving the 100% of enzymatic activity) and in the absence of enzyme (giving the baseline), were also included in each experiment. Reading was performed with a Microbeta Trilux (Perkin Elmer) luminometer, according to the manufacturer's protocol.

Human DDX3 helicase activity assay

The helicase activity of DDX3 wt and mutant forms was monitored by measuring the conversion of a double stranded (ds) DNA or RNA (labelled at the 5'-end of one strand with a 6-FAM fluorescent group or P^{32}, respectively) into single stranded (ss) nucleic acid. Reactions were performed in 50 mM TrisHCl pH 7.5, 1 mM DTT, 0.2 mg/ml BSA, 5% glycerol and 100 μM ATP, 10 mM $MgCl_2$ at 37°C degrees for 10' and stopped by adding EDTA 50 mM pH 8. Products were separated through non-denaturating 8%PAGE at 5 W for 2 hours in TBE buffer at 4°C. Substrates and products were quantified by laser scanning densitometry (Thyphoon-TRIO, GE Healthcare).

Kinetic analysis

ATPase reactions were performed as described, in the presence of increasing amounts of inhibitor and variable ATP concentrations. Variations of the initial velocities of the reaction as a function of ATP concentrations in the absence or presence of 4 were analyzed with the equation:

Eq. (1): $k_{cat} \cdot$ Eo/(l+(^s/[ATP]))

where k_{cat} is the reaction rate, Eo is the input enzyme concentration, [ATP] is the variable substrate concentration, K_S is the apparent affinity for the substrate. $K_S = K_m$ in the absence of the inhibitor, whereas $Ks = K_{m(app)}$ in the presence of the inhibitor.

Variation of the % inhibition as a function of compound FE15 at different ATP concentrations were fitted to the equation for cooperative binding:

Eq. (2): $V_{max} \cdot [If\ l(K_{i(app)} + [If)$

where V_{max} is the apparent maximal rate of the reaction in the absence of the inhibitor, [I] is the variable inhibitor concentration, n is the cooperativity index and $K_{i(app)}$ is the apparent inhibition constant. Comparatively, fitting was done with the same Eq. (2) where n was kept fixed at the value of 1 (non-cooperativity hypothesis). F test was used to compare the two fittings and p value was calculated.

The variation of the $K_{m(app)}$ as a function of the inhibitor concentration was fitted to the equation:

Eq. (3): $i\zeta_{m(app)} = KJ(\backslash + ([I]^n/K))$

The variation of the $K¾_{app)}$ as a function of the ATP substrate concentration was fitted to the equation:

Eq. (4): $K_{i(app)} = K \cdot (l + (i\zeta_m/[ATP])$

All values used are the means of at least three independent experiments.

Proteins

Human recombinant DDX3 was cloned, expressed and purified as described (Franca et al. *Proteins* **2007,** *67,* 1128-37).

Cell viability assays

Cell viability in the presence of the compounds has been determined by standard MTT assays.

Antiviral assays

The susceptibilities of HIV-1 recombinant strains to drugs was performed as follow.

In detail, 0.5 µg of each HIV-1 plasmid construct was transfected into $CD4^+$ HeLa cells by using the lipofectin reagent, according to the recommendations of the manufacturer (Invitrogen, Groningen, The Netherlands). After 3 days of incubation at 37°C, the cell supernatants, which contained reconstituted viable recombinant viruses, were collected.

Quantification of the newly produced recombinant strains was obtained by determination of the HIV RNA copy number in the cell culture supernatants. Successively, 10 ml of transfected HeLa $CD4^+$-cell culture supernatants containing wild-type, and mutated recombinant HIV strain RNA per ml, respectively, was used to infect aliquots of 10×10^6 phytohemagglutinin-stimulated peripheral blood mononuclear cells (PBMCs) from HIV-seronegative blood donors. After 4 h of incubation, supernatants were removed and infected PBMCs were incubated at 37°C in 10 ml of RPMI 1640 medium (Eurobio, Les Ulis Cedex B, France) supplemented with 20% fetal calf serum (Life Technologies, Ltd., Paisley, Scotland), 2 mM 1-glutamine, 100 U of penicillin per ml, 100 µg of streptomycin per ml, 10% interleukin-2 (ZeptoMetrix Co., Buffalo, N.Y.), 5 µg of hydrocortisone (Sigma Chemical Co.) per ml and with fourfold dilutions of antiretroviral drugs. No-drug controls for each drug dilution were included in each assay. After 3, 5 and 7 days of incubation the HIV-1 RNA in the cell culture supernatant was quantified. Recombinant HIV-1 strains from treatment-naive patients and multidrug resistance-associated changes were assayed in parallel. The degree of inhibition of viral replication was measured by determining the HIV-1 RNA level in the supernatants of cell cultures and was expressed as the fold increase in the 50% inhibitory concentrations (IC_{50}s) for resistant recombinant HIV-1 variants compared with the IC50S for the wild-type recombinant variant. Each test was performed in triplicate.

Modelling

Closed conformation of DDX3

The DDX3X(V168-G582) domain 2 has to rotate approximately 180° relative to domain 1 to obtain the closed conformation of the protein required for RNA binding. This rearrangement would bring positively charged patches on the solvent-exposed surface of domain 2 into closer proximity with positively charged surfaces on domain 1, thus forming the RNA-binding site of the protein.

A comparison of the closed structure of the VASA protein in complex with poly(U) with a modeled closed structure of the DDX3X(V168-G582) protein show that all amino acid residues that are involved in interaction with the RNA in the VASA-structure are present in the DDX3X(V168-G582) structure at corresponding positions. This indicates, as expected, that these residues are involved in RNA binding in both proteins, and that the RNA binding mode in this area should be very similar.

The present homology model has been built as follows: the "closed" structure was built by alignment of the individual domains on the respective domains of the protein eIF4A *(eukaryotic translation initiation factor)* which is in a closed conformation (pdb entry 2J0S, homology 37%) and final optimization of the resulting structure [RMS 1.2 **A].** 2J0S is cocrystallized with PolyU and this allowed the authors to immediately identify the binding site of nucleic acid for the authors' protein.

The alignment has been performend using Pymol alignement function. The structure obtained has been used as target for the authors' virtual docking studies. Protein Preparation Wizard procedure was used to obtain a satisfactory starting structure for docking studies. This facility is designed to ensure chemical correctness and to optimize the protein structure for further analysis. The process adds hydrogens, neutralizes appropriate amino acid chains, and relieves steric clashes. In particular, it performs a series of restrained, partial minimizations on the cocrystallized structure, each of which employs a limited number of minimization steps. It is not intended to minimize the system completely. In the present invention, the minimization (OPLS 2001 force field) was stopped when rmsd of the nonhydrogen atoms reached 0.30 **A.** The final homology model is reported in Appendix I.

APPENDIX I Structure coordinates of the Homology Model of DDX3 in the closed conformation reported in "PDB format" (for further detail see http://www.wwpdb.org/docs.html)

```
ATOM      1  N   MET A 167      19.061  73.704   3.313  1.00  0.00           N1+
ATOM      2  CA  MET A 167      18.817  74.581   2.164  1.00  0.00           C
ATOM      3  C   MET A 167      20.082  74.562   1.310  1.00  0.00           C
ATOM      4  O   MET A 167      20.140  73.825   0.328  1.00  0.00           O
ATOM      5  CB  MET A 167      18.358  75.990   2.588  1.00  0.00           C
ATOM      6  CG  MET A 167      18.124  76.936   1.403  1.00  0.00           C
ATOM      7  SD  MET A 167      16.981  76.327   0.132  1.00  0.00           S
ATOM      8  CE  MET A 167      17.039  77.716  -1.029  1.00  0.00           C
ATOM      9 1H   MET A 167      18.244  73.689   3.906  1.00  0.00           H
ATOM     10 2H   MET A 167      19.258  72.769   2.988  1.00  0.00           H
ATOM     11 3H   MET A 167      19.851  74.050   3.839  1.00  0.00           H
ATOM     12  HA  MET A 167      17.899  74.275   1.661  1.00  0.00           H
ATOM     13 1HB  MET A 167      17.421  75.917   3.139  1.00  0.00           H
ATOM     14 2HB  MET A 167      19.118  76.443   3.224  1.00  0.00           H
ATOM     15 1HG  MET A 167      17.709  77.877   1.765  1.00  0.00           H
ATOM     16 2HG  MET A 167      19.071  77.128   0.898  1.00  0.00           H
ATOM     17 1HE  MET A 167      16.388  77.508  -1.878  1.00  0.00           H
ATOM     18 2HE  MET A 167      16.703  78.624  -0.528  1.00  0.00           H
ATOM     19 3HE  MET A 167      18.061  77.854  -1.381  1.00  0.00           H
ATOM     20  N   VAL A 168      21.104  75.315   1.711  1.00  0.00           N
ATOM     21  CA  VAL A 168      22.421  75.342   1.104  1.00  0.00           C
ATOM     22  C   VAL A 168      23.409  75.495   2.265  1.00  0.00           C
ATOM     23  O   VAL A 168      23.614  76.603   2.758  1.00  0.00           O
ATOM     24  CB  VAL A 168      22.534  76.495   0.084  1.00  0.00           C
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ATOM   25 CGI VAL A 168    23.951 76.561  -0.505  1.00  0.00      C
ATOM   26 CG2 VAL A 168    21.550 76.321  -1.082  1.00  0.00      C
ATOM   27 H   VAL A 168    20.995 75.934   2.501  1.00  0.00      H
ATOM   28 HA  VAL A 168    22.578 74.427   0.532  1.00  0.00      H
ATOM   29 HB  VAL A 168    22.313 77.441   0.579  1.00  0.00      H
ATOM   30 1HG1 VAL A 168   24.009 77.381  -1.221  1.00  0.00      H
ATOM   31 2HG1 VAL A 168   24.671 76.728   0.297  1.00  0.00      H
ATOM   32 3HG1 VAL A 168   24.180 75.622  -1.009  1.00  0.00      H
ATOM   33 1HG2 VAL A 168   21.660 77.153  -1.778  1.00  0.00      H
ATOM   34 2HG2 VAL A 168   21.761 75.385  -1.599  1.00  0.00      H
ATOM   35 3HG2 VAL A 168   20.530 76.301  -0.698  1.00  0.00      H
ATOM   36 N   GLU A 169    24.029 74.393   2.689  1.00  0.00      N
ATOM   37 CA  GLU A 169    24.873 74.349   3.873  1.00  0.00      C
ATOM   38 C   GLU A 169    26.127 73.524   3.555  1.00  0.00      C
ATOM   39 O   GLU A 169    26.083 72.635   2.703  1.00  0.00      O
ATOM   40 CB  GLU A 169    24.099 73.754   5.066  1.00  0.00      C
ATOM   41 CG  GLU A 169    22.968 74.659   5.598  1.00  0.00      C
ATOM   42 CD  GLU A 169    21.610 74.412   4.957  1.00  0.00      C
ATOM   43 OE1 GLU A 169    21.021 75.337   4.368  1.00  0.00      O
ATOM   44 OE2 GLU A 169    21.080 73.287   5.025  1.00  0.00      Ol-
ATOM   45 H   GLU A 169    23.924 73.527   2.179  1.00  0.00      H
ATOM   46 HA  GLU A 169    25.124 75.364   4.179  1.00  0.00      H
ATOM   47 1HB  GLU A 169   23.641 72.810   4.769  1.00  0.00      H
ATOM   48 2HB  GLU A 169   24.786 73.579   5.894  1.00  0.00      H
ATOM   49 1HG  GLU A 169   22.847 74.498   6.670  1.00  0.00      H
ATOM   50 2HG  GLU A 169   23.220 75.703   5.414  1.00  0.00      H
ATOM   51 N   ALA A 170    27.248 73.811  4.225  1.00  0.00      N
ATOM   52 CA  ALA A 170    28.504 73.082  4.115  1.00  0.00      C
ATOM   53 C   ALA A 170    29.361 73.470   5.323  1.00  0.00      C
ATOM   54 O   ALA A 170    30.368 74.166   5.200  1.00  0.00      O
ATOM   55 CB  ALA A 170    29.202 73.423   2.793  1.00  0.00      C
ATOM   56 H   ALA A 170    27.266 74.589   4.868  1.00  0.00      H
ATOM   57 HA  ALA A 170    28.302 72.011  4.085  1.00  0.00      H
ATOM   58 1HB  ALA A 170   30.139 72.872   2.723  1.00  0.00      H
ATOM   59 2HB  ALA A 170   28.556 73.148   1.959  1.00  0.00      H
ATOM   60 3HB  ALA A 170   29.406 74.493   2.755  1.00  0.00      H
ATOM   61 N   THR A 171    28.932 73.047   6.506  1.00  0.00      N
ATOM   62 CA  THR A 171    29.159 73.776   7.735  1.00  0.00      C
ATOM   63 C   THR A 171    29.325 72.781   8.891  1.00  0.00      C
ATOM   64 O   THR A 171    28.515 71.871   9.058  1.00  0.00      O
ATOM   65 CB  THR A 171    27.929 74.681   7.966  1.00  0.00      C
ATOM   66 CG2 THR A 171    28.219 75.769   9.004  1.00  0.00      C
ATOM   67 OG1 THR A 171    27.509 75.308   6.760  1.00  0.00      O
ATOM   68 H   THR A 171    28.420 72.179   6.577  1.00  0.00      H
ATOM   69 HA  THR A 171    30.062 74.379   7.639  1.00  0.00      H
ATOM   70 HB  THR A 171    27.087 74.073   8.298  1.00  0.00      H
ATOM   71 1HG2 THR A 171   27.331 76.387   9.141  1.00  0.00      H
ATOM   72 2HG2 THR A 171   28.487 75.304   9.952  1.00  0.00      H
ATOM   73 3HG2 THR A 171   29.044 76.391   8.658  1.00  0.00      H
ATOM   74 HG1 THR A 171    26.745 75.861   6.936  1.00  0.00      H
ATOM   75 N   GLY A 172    30.358 72.950   9.712  1.00  0.00      N
ATOM   76 CA  GLY A 172    30.566 72.166  10.916  1.00  0.00      C
ATOM   77 C   GLY A 172    31.878 72.623  11.544  1.00  0.00      C
ATOM   78 O   GLY A 172    32.577 73.457  10.963  1.00  0.00      O
ATOM   79 H   GLY A 172    31.052 73.656   9.513  1.00  0.00      H
ATOM   80 1HA  GLY A 172   29.738 72.330  11.605  1.00  0.00      H
ATOM   81 2HA  GLY A 172   30.617 71.108  10.657  1.00  0.00      H
ATOM   82 N   ASN A 173    32.239 72.088  12.711  1.00  0.00      N
ATOM   83 CA  ASN A 173    33.562 72.353  13.261  1.00  0.00      C
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ATOM     84  C   ASN A 173      34.580  71.735  12.309  1.00  0.00           C
ATOM     85  O   ASN A 173      34.499  70.537  12.047  1.00  0.00           O
ATOM     86  CB  ASN A 173      33.737  71.708  14.638  1.00  0.00           C
ATOM     87  CG  ASN A 173      35.208  71.734  15.053  1.00  0.00           C
ATOM     88  ND2 ASN A 173      35.749  70.638  15.562  1.00  0.00           N
ATOM     89  OD1 ASN A 173      35.893  72.734  14.856  1.00  0.00           O
ATOM     90  H   ASN A 173      31.595  71.498  13.217  1.00  0.00           H
ATOM     91  HA  ASN A 173      33.726  73.429  13.314  1.00  0.00           H
ATOM     92  1HB ASN A 173      33.150  72.257  15.375  1.00  0.00           H
ATOM     93  2HB ASN A 173      33.396  70.673  14.601  1.00  0.00           H
ATOM     94  1HD2 ASN A 173      36.719  70.637  15.841  1.00  0.00          H
ATOM     95  2HD2 ASN A 173      35.191  69.803  15.671  1.00  0.00          H
ATOM     96  N   ASN A 174      35.544  72.518  11.827  1.00  0.00           N
ATOM     97  CA  ASN A 174      36.570  72.057  10.902  1.00  0.00           C
ATOM     98  C   ASN A 174      35.911  71.331  9.728  1.00  0.00           C
ATOM     99  O   ASN A 174      36.057  70.119  9.567  1.00  0.00           O
ATOM     100  CB  ASN A 174      37.616  71.191  11.625  1.00  0.00          C
ATOM     101  CG  ASN A 174      38.664  72.043  12.331  1.00  0.00          C
ATOM     102  ND2 ASN A 174      38.362  72.575  13.510  1.00  0.00          N
ATOM     103  OD1 ASN A 174      39.753  72.250  11.809  1.00  0.00          O
ATOM     104  H   ASN A 174      35.589  73.489  12.101  1.00  0.00           H
ATOM     105  HA  ASN A 174      37.192  72.900  10.598  1.00  0.00           H
ATOM     106  1HB ASN A 174      37.120  70.570  12.371  1.00  0.00           H
ATOM     107  2HB ASN A 174      38.124  70.554  10.901  1.00  0.00           H
ATOM     108  1HD2 ASN A 174      39.041  73.143  13.996  1.00  0.00          H
ATOM     109  2HD2 ASN A 174      37.454  72.412  13.920  1.00  0.00          H
ATOM     110  N   CYS A 175      35.191  72.098  8.909  1.00  0.00           N
ATOM     111  CA  CYS A 175      34.717  71.648  7.610  1.00  0.00           C
ATOM     112  C   CYS A 175      35.952  71.585  6.701  1.00  0.00           C
ATOM     113  O   CYS A 175      36.671  72.580  6.619  1.00  0.00           O
ATOM     114  CB  CYS A 175      33.672  72.639  7.082  1.00  0.00           C
ATOM     115  SG  CYS A 175      32.855  71.965  5.610  1.00  0.00           S
ATOM     116  H   CYS A 175      34.950  73.040  9.182  1.00  0.00           H
ATOM     117  HA  CYS A 175      34.244  70.672  7.714  1.00  0.00           H
ATOM     118  1HB CYS A 175      32.923  72.823  7.852  1.00  0.00           H
ATOM     119  2HB CYS A 175      34.160  73.578  6.820  1.00  0.00           H
ATOM     120  HG  CYS A 175      32.109  72.685  5.242  1.00  0.00           H
ATOM     121  N   PRO A 176      36.255  70.451  6.057  1.00  0.00           N
ATOM     122  CA  PRO A 176      37.606  70.223  5.565  1.00  0.00           C
ATOM     123  C   PRO A 176      37.812  70.803  4.157  1.00  0.00           C
ATOM     124  O   PRO A 176      36.854  70.934  3.392  1.00  0.00           O
ATOM     125  CB  PRO A 176      37.776  68.698  5.558  1.00  0.00           C
ATOM     126  CG  PRO A 176      36.351  68.181  5.382  1.00  0.00           C
ATOM     127  CD  PRO A 176      35.542  69.192  6.190  1.00  0.00           C
ATOM     128  HA  PRO A 176      38.323  70.690  6.240  1.00  0.00           H
ATOM     129  1HB PRO A 176      38.428  68.408  4.734  1.00  0.00           H
ATOM     130  2HB PRO A 176      38.220  68.377  6.501  1.00  0.00           H
ATOM     131  1HG PRO A 176      36.094  68.178  4.323  1.00  0.00           H
ATOM     132  2HG PRO A 176      36.281  67.167  5.775  1.00  0.00           H
ATOM     133  1HD PRO A 176      35.492  68.912  7.242  1.00  0.00           H
ATOM     134  2HD PRO A 176      34.533  69.302  5.795  1.00  0.00           H
ATOM     135  N   PRO A 177      39.061  71.128  3.779  1.00  0.00           N
ATOM     136  CA  PRO A 177      39.388  71.329  2.376  1.00  0.00           C
ATOM     137  C   PRO A 177      38.974  70.105  1.546  1.00  0.00           C
ATOM     138  O   PRO A 177      38.903  68.988  2.060  1.00  0.00           O
ATOM     139  CB  PRO A 177      40.903  71.537  2.345  1.00  0.00           C
ATOM     140  CG  PRO A 177      41.389  70.682  3.514  1.00  0.00           C
ATOM     141  CD  PRO A 177      40.266  70.835  4.541  1.00  0.00           C
ATOM     142  HA  PRO A 177      38.863  72.208  2.003  1.00  0.00           H
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ATOM   143 IHB  PRO A 177      41.297  71.200   1.386  1.00  0.00           H
ATOM   144 2HB  PRO A 177      41.128  72.596   2.477  1.00  0.00           H
ATOM   145 IHG  PRO A 177      41.517  69.652   3.183  1.00  0.00           H
ATOM   146 2HG  PRO A 177      42.343  71.068   3.876  1.00  0.00           H
ATOM   147 1HD  PRO A 177      40.471  71.657   5.228  1.00  0.00           H
ATOM   148 2HD  PRO A 177      40.124  69.915   5.108  1.00  0.00           H
ATOM   149  N   HIS A 178      38.710  70.318   0.258  1.00  0.00           N
ATOM   150  CA  HIS A 178      38.026  69.341  -0.571  1.00  0.00           C
ATOM   151  C   HIS A 178      38.954  68.753  -1.633  1.00  0.00           C
ATOM   152  O   HIS A 178      39.988  69.339  -1.944  1.00  0.00           O
ATOM   153  CB  HIS A 178      36.760  69.970  -1.163  1.00  0.00           C
ATOM   154  CG  HIS A 178      36.913  71.164  -2.070  1.00  0.00           C
ATOM   155  CD2 HIS A 178      37.856  71.534  -2.998  1.00  0.00           C
ATOM   156  ND1 HIS A 178      35.944  72.159  -2.127  1.00  0.00           N
ATOM   157  CE1 HIS A 178      36.286  73.030  -3.088  1.00  0.00           C
ATOM   158  NE2 HIS A 178      37.405  72.642  -3.701  1.00  0.00           N
ATOM   159  H   HIS A 178      38.987  71.186  -0.178  1.00  0.00           H
ATOM   160  HA  HIS A 178      37.568  68.582   0.063  1.00  0.00           H
ATOM   161 IHB  HIS A 178      36.231  69.229  -1.762  1.00  0.00           H
ATOM   162 2HB  HIS A 178      36.112  70.312  -0.356  1.00  0.00           H
ATOM   163  HD2 HIS A 178      38.776  70.975  -3.085  1.00  0.00           H
ATOM   164  HD1 HIS A 178      35.153  72.129  -1.499  1.00  0.00           H
ATOM   165  HE1 HIS A 178      35.675  73.902  -3.270  1.00  0.00           H
ATOM   166  N   ILE A 179      38.573  67.609  -2.205  1.00  0.00           N
ATOM   167  CA  ILE A 179      39.376  66.922  -3.213  1.00  0.00           C
ATOM   168  C   ILE A 179      38.980  67.431  -4.606  1.00  0.00           C
ATOM   169  O   ILE A 179      38.197  68.382  -4.701  1.00  0.00           O
ATOM   170  CB  ILE A 179      39.214  65.400  -3.052  1.00  0.00           C
ATOM   171  CGI ILE A 179      37.799  64.906  -3.406  1.00  0.00           C
ATOM   172  CG2 ILE A 179      39.636  64.967  -1.640  1.00  0.00           C
ATOM   173  CD1 ILE A 179      37.785  63.396  -3.646  1.00  0.00           C
ATOM   174  H   ILE A 179      37.696  67.181  -1.944  1.00  0.00           H
ATOM   175  HA  ILE A 179      40.434  67.055  -2.989  1.00  0.00           H
ATOM   176  HB  ILE A 179      39.987  64.889  -3.626  1.00  0.00           H
ATOM   177 1HG1 ILE A 179      37.118  65.134  -2.585  1.00  0.00           H
ATOM   178 2HG1 ILE A 179      37.455  65.406  -4.311  1.00  0.00           H
ATOM   179 1HG2 ILE A 179      39.516  63.888  -1.539  1.00  0.00           H
ATOM   180 2HG2 ILE A 179      40.680  65.234  -1.474  1.00  0.00           H
ATOM   181 3HG2 ILE A 179      39.011  65.472  -0.903  1.00  0.00           H
ATOM   182 1HD1 ILE A 179      36.773  63.076  -3.894  1.00  0.00           H
ATOM   183 2HD1 ILE A 179      38.455  63.153  -4.472  1.00  0.00           H
ATOM   184 3HD1 ILE A 179      38.118  62.881  -2.745  1.00  0.00           H
ATOM   185  N   GLU A 180      39.463  66.811  -5.688  1.00  0.00           N
ATOM   186  CA  GLU A 180      39.273  67.302  -7.047  1.00  0.00           C
ATOM   187  C   GLU A 180      38.872  66.196  -8.028  1.00  0.00           C
ATOM   188  O   GLU A 180      38.253  66.499  -9.054  1.00  0.00           O
ATOM   189  CB  GLU A 180      40.559  68.005  -7.508  1.00  0.00           C
ATOM   190  CG  GLU A 180      40.514  69.513  -7.221  1.00  0.00           C
ATOM   191  CD  GLU A 180      39.640  70.206  -8.245  1.00  0.00           C
ATOM   192  OE1 GLU A 180      40.110  70.374  -9.388  1.00  0.00           O
ATOM   193  OE2 GLU A 180      38.448  70.448  -7.962  1.00  0.00           Ol-
ATOM   194  H   GLU A 180      39.990  65.956  -5.586  1.00  0.00           H
ATOM   195  HA  GLU A 180      38.531  68.100  -7.045  1.00  0.00           H
ATOM   196 IHB  GLU A 180      41.414  67.581  -6.981  1.00  0.00           H
ATOM   197 2HB  GLU A 180      40.687  67.863  -8.581  1.00  0.00           H
ATOM   198 IHG  GLU A 180      40.104  69.683  -6.225  1.00  0.00           H
ATOM   199 2HG  GLU A 180      41.522  69.924  -7.273  1.00  0.00           H
ATOM   200  N   SER A 181      39.221  64.942  -7.752  1.00  0.00           N
ATOM   201  CA  SER A 181      39.054  63.848  -8.696  1.00  0.00           C
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ATOM    202  C   SER A 181     38.513  62.594  -7.992  1.00  0.00           C
ATOM    203  O   SER A 181     37.561  62.698  -7.218  1.00  0.00           O
ATOM    204  CB  SER A 181     40.368  63.656  -9.466  1.00  0.00           C
ATOM    205  OG  SER A 181     40.762  64.882 -10.060  1.00  0.00           O
ATOM    206  H   SER A 181     39.621  64.716  -6.853  1.00  0.00           H
ATOM    207  HA  SER A 181     38.464  64.189  -9.547  1.00  0.00           H
ATOM    208 1HB  SER A 181     41.147  63.323  -8.780  1.00  0.00           H
ATOM    209 2HB  SER A 181     40.227  62.908 -10.246  1.00  0.00           H
ATOM    210  HG  SER A 181     41.584  64.756 -10.540  1.00  0.00           H
ATOM    211  N   PHE A 182     39.046  61.405  -8.291  1.00  0.00           N
ATOM    212  CA  PHE A 182     38.544  60.132  -7.786  1.00  0.00           C
ATOM    213  C   PHE A 182     39.745  59.216  -7.549  1.00  0.00           C
ATOM    214  O   PHE A 182     39.709  58.016  -7.819  1.00  0.00           O
ATOM    215  CB  PHE A 182     37.596  59.488  -8.809  1.00  0.00           C
ATOM    216  CG  PHE A 182     36.305  60.221  -9.120  1.00  0.00           C
ATOM    217  CD1 PHE A 182     35.372  60.500  -8.101  1.00  0.00           C
ATOM    218  CD2 PHE A 182     35.995  60.596 -10.442  1.00  0.00           C
ATOM    219  CE1 PHE A 182     34.135  61.095  -8.402  1.00  0.00           C
ATOM    220  CE2 PHE A 182     34.764  61.202 -10.744  1.00  0.00           C
ATOM    221  CZ  PHE A 182     33.825  61.437  -9.728  1.00  0.00           C
ATOM    222  H   PHE A 182     39.848  61.350  -8.902  1.00  0.00           H
ATOM    223  HA  PHE A 182     38.008  60.297  -6.852  1.00  0.00           H
ATOM    224 1HB  PHE A 182     38.108  59.386  -9.766  1.00  0.00           H
ATOM    225 2HB  PHE A 182     37.291  58.504  -8.453  1.00  0.00           H
ATOM    226  HDl PHE A 182     35.604  60.255  -7.075  1.00  0.00           H
ATOM    227  HD2 PHE A 182     36.707  60.418 -11.234  1.00  0.00           H
ATOM    228  HE1 PHE A 182     33.423  61.289  -7.614  1.00  0.00           H
ATOM    229  HE2 PHE A 182     34.538  61.488 -11.760  1.00  0.00           H
ATOM    230  HZ  PHE A 182     32.867  61.879  -9.962  1.00  0.00           H
ATOM    231  N   SER A 183     40.834  59.813  -7.092  1.00  0.00           N
ATOM    232  CA  SER A 183     42.171  59.253  -7.081  1.00  0.00           C
ATOM    233  C   SER A 183     42.877  59.637  -5.777  1.00  0.00           C
ATOM    234  O   SER A 183     44.046  59.317  -5.580  1.00  0.00           O
ATOM    235  CB  SER A 183     42.917  59.848  -8.290  1.00  0.00           C
ATOM    236  OG  SER A 183     42.297  61.049  -8.741  1.00  0.00           O
ATOM    237  H   SER A 183     40.776  60.744  -6.707  1.00  0.00           H
ATOM    238  HA  SER A 183     42.111  58.166  -7.147  1.00  0.00           H
ATOM    239 1HB  SER A 183     43.945  60.075  -8.007  1.00  0.00           H
ATOM    240 2HB  SER A 183     42.916  59.129  -9.109  1.00  0.00           H
ATOM    241  HG  SER A 183     42.782  61.397  -9.493  1.00  0.00           H
ATOM    242  N   ASP A 184     42.187  60.408  -4.938  1.00  0.00           N
ATOM    243  CA  ASP A 184     42.820  61.525  -4.255  1.00  0.00           C
ATOM    244  C   ASP A 184     43.260  61.116  -2.839  1.00  0.00           C
ATOM    245  O   ASP A 184     43.665  61.964  -2.051  1.00  0.00           O
ATOM    246  CB  ASP A 184     41.847  62.729  -4.249  1.00  0.00           C
ATOM    247  CG  ASP A 184     41.400  63.229  -5.628  1.00  0.00           C
ATOM    248  OD1 ASP A 184     41.348  62.406  -6.568  1.00  0.00           O
ATOM    249  OD2 ASP A 184     41.035  64.420  -5.744  1.00  0.00           Ol-
ATOM    250  H   ASP A 184     41.209  60.220  -4.768  1.00  0.00           H
ATOM    251  HA  ASP A 184     43.652  61.894  -4.855  1.00  0.00           H
ATOM    252 1HB  ASP A 184     40.937  62.459  -3.713  1.00  0.00           H
ATOM    253 2HB  ASP A 184     42.320  63.578  -3.755  1.00  0.00           H
ATOM    254  N   VAL A 185     43.171  59.818  -2.523  1.00  0.00           N
ATOM    255  CA  VAL A 185     43.515  59.163  -1.259  1.00  0.00           C
ATOM    256  C   VAL A 185     43.609  57.651  -1.556  1.00  0.00           C
ATOM    257  O   VAL A 185     43.545  57.275  -2.730  1.00  0.00           O
ATOM    258  CB  VAL A 185     42.475  59.472  -0.153  1.00  0.00           C
ATOM    259  CGI VAL A 185     42.580  60.897   0.405  1.00  0.00           C
ATOM    260  CG2 VAL A 185     41.030  59.213  -0.600  1.00  0.00           C
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ATOM    261  H   VAL A 185      42.829  59.155  -3.204  1.00  0.00           H
ATOM    262  HA  VAL A 185      44.445  59.580  -0.874  1.00  0.00           H
ATOM    263  HB  VAL A 185      42.556  58.730   0.640  1.00  0.00           H
ATOM    264 1HG1 VAL A 185      41.822  61.043   1.175  1.00  0.00           H
ATOM    265 2HG1 VAL A 185      43.569  61.046   0.838  1.00  0.00           H
ATOM    266 3HG1 VAL A 185      42.424  61.616  -0.399  1.00  0.00           H
ATOM    267 1HG2 VAL A 185      40.348  59.448   0.217  1.00  0.00           H
ATOM    268 2HG2 VAL A 185      40.796  59.841  -1.460  1.00  0.00           H
ATOM    269 3HG2 VAL A 185      40.917  58.164  -0.876  1.00  0.00           H
ATOM    270  N   GLU A 186      43.739  56.768  -0.553  1.00  0.00           N
ATOM    271  CA  GLU A 186      43.956  55.342  -0.780  1.00  0.00           C
ATOM    272  C   GLU A 186      42.799  54.737  -1.586  1.00  0.00           C
ATOM    273  O   GLU A 186      41.740  54.418  -1.041  1.00  0.00           O
ATOM    274  CB  GLU A 186      44.152  54.543   0.522  1.00  0.00           C
ATOM    275  CG  GLU A 186      45.092  55.183   1.552  1.00  0.00           C
ATOM    276  CD  GLU A 186      44.273  55.982   2.538  1.00  0.00           C
ATOM    277  OE1 GLU A 186      43.834  57.077   2.145  1.00  0.00           O
ATOM    278  OE2 GLU A 186      43.895  55.433   3.596  1.00  0.00           Ol-
ATOM    279  H   GLU A 186      43.688  57.082   0.406  1.00  0.00           H
ATOM    280  HA  GLU A 186      44.914  55.195  -1.280  1.00  0.00           H
ATOM    281 1HB  GLU A 186      43.190  54.417   1.020  1.00  0.00           H
ATOM    282 2HB  GLU A 186      44.571  53.564   0.289  1.00  0.00           H
ATOM    283 1HG  GLU A 186      45.640  54.402   2.079  1.00  0.00           H
ATOM    284 2HG  GLU A 186      45.796  55.841   1.043  1.00  0.00           H
ATOM    285  N   MET A 187      43.019  54.553  -2.883  1.00  0.00           N
ATOM    286  CA  MET A 187      42.015  54.197  -3.867  1.00  0.00           C
ATOM    287  C   MET A 187      42.792  53.744  -5.098  1.00  0.00           C
ATOM    288  O   MET A 187      42.866  52.553  -5.396  1.00  0.00           O
ATOM    289  CB  MET A 187      41.114  55.404  -4.201  1.00  0.00           C
ATOM    290  CG  MET A 187      40.115  55.763  -3.093  1.00  0.00           C
ATOM    291  SD  MET A 187      38.765  56.880  -3.567  1.00  0.00           S
ATOM    292  CE  MET A 187      39.719  58.291  -4.177  1.00  0.00           C
ATOM    293  H   MET A 187      43.951  54.660  -3.257  1.00  0.00           H
ATOM    294  HA  MET A 187      41.388  53.397  -3.474  1.00  0.00           H
ATOM    295 1HB  MET A 187      41.733  56.285  -4.373  1.00  0.00           H
ATOM    296 2HB  MET A 187      40.534  55.188  -5.099  1.00  0.00           H
ATOM    297 1HG  MET A 187      39.639  54.855  -2.724  1.00  0.00           H
ATOM    298 2HG  MET A 187      40.641  56.255  -2.275  1.00  0.00           H
ATOM    299 1HE  MET A 187      39.037  59.074  -4.509  1.00  0.00           H
ATOM    300 2HE  MET A 187      40.351  58.676  -3.376  1.00  0.00           H
ATOM    301 3HE  MET A 187      40.343  57.974  -5.012  1.00  0.00           H
ATOM    302  N   GLY A 188      43.423  54.707  -5.775  1.00  0.00           N
ATOM    303  CA  GLY A 188      44.259  54.473  -6.938  1.00  0.00           C
ATOM    304  C   GLY A 188      43.602  53.496  -7.914  1.00  0.00           C
ATOM    305  O   GLY A 188      42.441  53.675  -8.277  1.00  0.00           O
ATOM    306  H   GLY A 188      43.333  55.670  -5.484  1.00  0.00           H
ATOM    307 1HA  GLY A 188      44.431  55.416  -7.458  1.00  0.00           H
ATOM    308 2HA  GLY A 188      45.214  54.054  -6.621  1.00  0.00           H
ATOM    309  N   GLU A 189      44.351  52.471  -8.327  1.00  0.00           N
ATOM    310  CA  GLU A 189      43.938  51.434  -9.264  1.00  0.00           C
ATOM    311  C   GLU A 189      42.536  50.908  -8.928  1.00  0.00           C
ATOM    312  O   GLU A 189      41.707  50.685  -9.812  1.00  0.00           O
ATOM    313  CB  GLU A 189      44.992  50.311  -9.214  1.00  0.00           C
ATOM    314  CG  GLU A 189      45.132  49.536 -10.529  1.00  0.00           C
ATOM    315  CD  GLU A 189      43.867  48.796 -10.913  1.00  0.00           C
ATOM    316  OE1 GLU A 189      43.566  48.744 -12.121  1.00  0.00           O
ATOM    317  OE2 GLU A 189      43.172  48.286 -10.012  1.00  0.00           Ol-
ATOM    318  H   GLU A 189      45.295  52.365  -7.985  1.00  0.00           H
ATOM    319  HA  GLU A 189      43.966  51.830 -10.280  1.00  0.00           H
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ATOM    320 IHB  GLU A 189      45.968  50.738  -8.985  1.00  0.00           H
ATOM    321 2HB  GLU A 189      44.720  49.591  -8.442  1.00  0.00           H
ATOM    322 IHG  GLU A 189      45.369  50.229 -11.336  1.00  0.00           H
ATOM    323 2HG  GLU A 189      45.931  48.801 -10.435  1.00  0.00           H
ATOM    324  N   ILE A 190      42.264  50.706  -7.639  1.00  0.00           N
ATOM    325  CA  ILE A 190      41.107  49.941  -7.210  1.00  0.00           C
ATOM    326  C   ILE A 190      39.827  50.736  -7.504  1.00  0.00           C
ATOM    327  O   ILE A 190      38.729  50.178  -7.510  1.00  0.00           O
ATOM    328  CB  ILE A 190      41.248  49.523  -5.728  1.00  0.00           C
ATOM    329  CGI ILE A 190      42.669  49.001  -5.420  1.00  0.00           C
ATOM    330  CG2 ILE A 190      40.225  48.424  -5.404  1.00  0.00           C
ATOM    331  CD1 ILE A 190      42.857  48.537  -3.971  1.00  0.00           C
ATOM    332  H   ILE A 190      42.871  51.090  -6.929  1.00  0.00           H
ATOM    333  HA  ILE A 190      41.134  48.952  -7.669  1.00  0.00           H
ATOM    334  HB  ILE A 190      41.033  50.379  -5.088  1.00  0.00           H
ATOM    335 1HG1 ILE A 190      42.891  48.150  -6.064  1.00  0.00           H
ATOM    336 2HG1 ILE A 190      43.395  49.793  -5.602  1.00  0.00           H
ATOM    337 1HG2 ILE A 190      40.325  48.131  -4.359  1.00  0.00           H
ATOM    338 2HG2 ILE A 190      39.218  48.801  -5.580  1.00  0.00           H
ATOM    339 3HG2 ILE A 190      40.406  47.559  -6.042  1.00  0.00           H
ATOM    340 1HD1 ILE A 190      43.878  48.184  -3.832  1.00  0.00           H
ATOM    341 2HD1 ILE A 190      42.665  49.369  -3.295  1.00  0.00           H
ATOM    342 3HD1 ILE A 190      42.160  47.726  -3.756  1.00  0.00           H
ATOM    343  N   ILE A 191      39.964  52.035  -7.771  1.00  0.00           N
ATOM    344  CA  ILE A 191      38.884  52.892  -8.218  1.00  0.00           C
ATOM    345  C   ILE A 191      39.142  53.270  -9.674  1.00  0.00           C
ATOM    346  O   ILE A 191      38.284  53.043 -10.521  1.00  0.00           O
ATOM    347  CB  ILE A 191      38.747  54.112  -7.292  1.00  0.00           C
ATOM    348  CGI ILE A 191      38.412  53.699  -5.844  1.00  0.00           C
ATOM    349  CG2 ILE A 191      37.710  55.114  -7.821  1.00  0.00           C
ATOM    350  CD1 ILE A 191      37.130  52.876  -5.673  1.00  0.00           C
ATOM    351  H   ILE A 191      40.865  52.480  -7.666  1.00  0.00           H
ATOM    352  HA  ILE A 191      37.931  52.387  -8.060  1.00  0.00           H
ATOM    353  HB  ILE A 191      39.656  54.711  -7.342  1.00  0.00           H
ATOM    354 1HG1 ILE A 191      39.222  53.091  -5.442  1.00  0.00           H
ATOM    355 2HG1 ILE A 191      38.288  54.591  -5.230  1.00  0.00           H
ATOM    356 1HG2 ILE A 191      37.642  55.962  -7.140  1.00  0.00           H
ATOM    357 2HG2 ILE A 191      38.013  55.464  -8.808  1.00  0.00           H
ATOM    358 3HG2 ILE A 191      36.737  54.627  -7.892  1.00  0.00           H
ATOM    359 1HD1 ILE A 191      36.988  52.639  -4.619  1.00  0.00           H
ATOM    360 2HD1 ILE A 191      36.278  53.452  -6.034  1.00  0.00           H
ATOM    361 3HD1 ILE A 191      37.212  51.952  -6.246  1.00  0.00           H
ATOM    362  N   MET A 192      40.305  53.847  -9.972  1.00  0.00           N
ATOM    363  CA  MET A 192      40.636  54.366 -11.292  1.00  0.00           C
ATOM    364  C   MET A 192      40.480  53.279 -12.354  1.00  0.00           C
ATOM    365  O   MET A 192      39.865  53.508 -13.392  1.00  0.00           O
ATOM    366  CB  MET A 192      42.055  54.949 -11.301  1.00  0.00           C
ATOM    367  CG  MET A 192      42.188  56.192 -10.409  1.00  0.00           C
ATOM    368  SD  MET A 192      41.172  57.628 -10.858  1.00  0.00           S
ATOM    369  CE  MET A 192      41.852  58.040 -12.487  1.00  0.00           C
ATOM    370  H   MET A 192      41.018  53.945  -9.263  1.00  0.00           H
ATOM    371  HA  MET A 192      40.013  55.234 -11.508  1.00  0.00           H
ATOM    372 IHB  MET A 192      42.758  54.200 -10.938  1.00  0.00           H
ATOM    373 2HB  MET A 192      42.323  55.237 -12.318  1.00  0.00           H
ATOM    374 IHG  MET A 192      41.907  55.939  -9.387  1.00  0.00           H
ATOM    375 2HG  MET A 192      43.220  56.543 -10.425  1.00  0.00           H
ATOM    376 1HE  MET A 192      41.327  58.905 -12.892  1.00  0.00           H
ATOM    377 2HE  MET A 192      42.912  58.272 -12.390  1.00  0.00           H
ATOM    378 3HE  MET A 192      41.725  57.192 -13.159  1.00  0.00           H
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ATOM    379  N   GLY A 193      40.974  52.076 -12.075  1.00  0.00           N
ATOM    380  CA  GLY A 193      40.907  50.950 -12.992  1.00  0.00           C
ATOM    381  C   GLY A 193      39.532  50.282 -12.944  1.00  0.00           C
ATOM    382  O   GLY A 193      39.355  49.169 -13.433  1.00  0.00           O
ATOM    383  H   GLY A 193      41.424  51.909 -11.187  1.00  0.00           H
ATOM    384  1HA GLY A 193      41.089  51.298 -14.009  1.00  0.00           H
ATOM    385  2HA GLY A 193      41.662  50.213 -12.720  1.00  0.00           H
ATOM    386  N   ASN A 194      38.550  50.952 -12.340  1.00  0.00           N
ATOM    387  CA  ASN A 194      37.149  50.575 -12.332  1.00  0.00           C
ATOM    388  C   ASN A 194      36.312  51.769 -12.808  1.00  0.00           C
ATOM    389  O   ASN A 194      35.100  51.644 -12.995  1.00  0.00           O
ATOM    390  CB  ASN A 194      36.739  50.126 -10.921  1.00  0.00           C
ATOM    391  CG  ASN A 194      37.197  48.705 -10.599  1.00  0.00           C
ATOM    392  ND2 ASN A 194      37.734  48.452  -9.406  1.00  0.00           N
ATOM    393  OD1 ASN A 194      37.103  47.806 -11.423  1.00  0.00           O
ATOM    394  H   ASN A 194      38.755  51.800 -11.832  1.00  0.00           H
ATOM    395  HA  ASN A 194      37.003  49.701 -12.967  1.00  0.00           H
ATOM    396  1HB ASN A 194      37.183  50.795 -10.183  1.00  0.00           H
ATOM    397  2HB ASN A 194      35.653  50.155 -10.831  1.00  0.00           H
ATOM    398  1HD2 ASN A 194      38.042  47.518  -9.178  1.00  0.00           H
ATOM    399  2HD2 ASN A 194      37.834  49.196  -8.729  1.00  0.00           H
ATOM    400  N   ILE A 195      36.926  52.933 -13.059  1.00  0.00           N
ATOM    401  CA  ILE A 195      36.215  54.053 -13.658  1.00  0.00           C
ATOM    402  C   ILE A 195      35.805  53.659 -15.076  1.00  0.00           C
ATOM    403  O   ILE A 195      34.788  54.138 -15.569  1.00  0.00           O
ATOM    404  CB  ILE A 195      37.019  55.371 -13.598  1.00  0.00           C
ATOM    405  CGI ILE A 195      37.060  55.861 -12.140  1.00  0.00           C
ATOM    406  CG2 ILE A 195      36.400  56.467 -14.481  1.00  0.00           C
ATOM    407  CD1 ILE A 195      37.848  57.159 -11.954  1.00  0.00           C
ATOM    408  H   ILE A 195      37.904  53.047 -12.832  1.00  0.00           H
ATOM    409  HA  ILE A 195      35.395  54.354 -13.007  1.00  0.00           H
ATOM    410  HB  ILE A 195      38.029  55.198 -13.969  1.00  0.00           H
ATOM    411  1HG1 ILE A 195      36.044  56.044 -11.789  1.00  0.00           H
ATOM    412  2HG1 ILE A 195      37.529  55.103 -11.514  1.00  0.00           H
ATOM    413  1HG2 ILE A 195      36.999  57.375 -14.407  1.00  0.00           H
ATOM    414  2HG2 ILE A 195      36.378  56.131 -15.517  1.00  0.00           H
ATOM    415  3HG2 ILE A 195      35.384  56.674 -14.145  1.00  0.00           H
ATOM    416  1HD1 ILE A 195      37.834  57.445 -10.902  1.00  0.00           H
ATOM    417  2HD1 ILE A 195      38.878  57.009 -12.275  1.00  0.00           H
ATOM    418  3HD1 ILE A 195      37.393  57.950 -12.551  1.00  0.00           H
ATOM    419  N   GLU A 196      36.527  52.740 -15.714  1.00  0.00           N
ATOM    420  CA  GLU A 196      36.171  52.244 -17.033  1.00  0.00           C
ATOM    421  C   GLU A 196      34.872  51.419 -17.009  1.00  0.00           C
ATOM    422  O   GLU A 196      34.374  51.010 -18.061  1.00  0.00           O
ATOM    423  CB  GLU A 196      37.356  51.464 -17.619  1.00  0.00           C
ATOM    424  CG  GLU A 196      38.440  52.431 -18.121  1.00  0.00           C
ATOM    425  CD  GLU A 196      37.953  53.147 -19.368  1.00  0.00           C
ATOM    426  OE1 GLU A 196      37.883  52.471 -20.414  1.00  0.00           O
ATOM    427  OE2 GLU A 196      37.444  54.278 -19.250  1.00  0.00           Ol-
ATOM    428  H   GLU A 196      37.358  52.361 -15.282  1.00  0.00           H
ATOM    429  HA  GLU A 196      36.124  53.077 -17.735  1.00  0.00           H
ATOM    430  1HB GLU A 196      37.783  50.821 -16.850  1.00  0.00           H
ATOM    431  2HB GLU A 196      37.012  50.854 -18.454  1.00  0.00           H
ATOM    432  IHG GLU A 196      38.659  53.166 -17.346  1.00  0.00           H
ATOM    433  2HG GLU A 196      39.345  51.872 -18.356  1.00  0.00           H
ATOM    434  N   LEU A 197      34.289  51.199 -15.829  1.00  0.00           N
ATOM    435  CA  LEU A 197      32.974  50.596 -15.671  1.00  0.00           C
ATOM    436  C   LEU A 197      31.936  51.695 -15.409  1.00  0.00           C
ATOM    437  O   LEU A 197      30.807  51.395 -15.029  1.00  0.00           O
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ATOM    438  CB  LEU A 197      32.996  49.589 -14.509  1.00  0.00           C
ATOM    439  CG  LEU A 197      34.124  48.547 -14.601  1.00  0.00           C
ATOM    440  CD1 LEU A 197      34.105  47.668 -13.347  1.00  0.00           C
ATOM    441  CD2 LEU A 197      33.985  47.663 -15.846  1.00  0.00           C
ATOM    442  H   LEU A 197      34.765  51.456 -14.975  1.00  0.00           H
ATOM    443  HA  LEU A 197      32.721  50.034 -16.570  1.00  0.00           H
ATOM    444 1HB  LEU A 197      33.130  50.123 -13.567  1.00  0.00           H
ATOM    445 2HB  LEU A 197      32.055  49.041 -14.484  1.00  0.00           H
ATOM    446  HG  LEU A 197      35.083  49.056 -14.701  1.00  0.00           H
ATOM    447 1HD1 LEU A 197      34.903  46.928 -13.409  1.00  0.00           H
ATOM    448 2HD1 LEU A 197      34.255  48.290 -12.465  1.00  0.00           H
ATOM    449 3HD1 LEU A 197      33.144  47.160 -13.273  1.00  0.00           H
ATOM    450 1HD2 LEU A 197      34.802  46.941 -15.873  1.00  0.00           H
ATOM    451 2HD2 LEU A 197      33.033  47.133 -15.812  1.00  0.00           H
ATOM    452 3HD2 LEU A 197      34.022  48.285 -16.741  1.00  0.00           H
ATOM    453  N   THR A 198      32.324  52.967 -15.562  1.00  0.00           N
ATOM    454  CA  THR A 198      31.583  54.099 -15.025  1.00  0.00           C
ATOM    455  C   THR A 198      31.760  55.357 -15.892  1.00  0.00           C
ATOM    456  O   THR A 198      30.857  55.729 -16.634  1.00  0.00           O
ATOM    457  CB  THR A 198      32.019  54.335 -13.564  1.00  0.00           C
ATOM    458  CG2 THR A 198      31.038  55.274 -12.866  1.00  0.00           C
ATOM    459  OG1 THR A 198      32.080  53.126 -12.834  1.00  0.00           O
ATOM    460  H   THR A 198      33.169  53.179 -16.073  1.00  0.00           H
ATOM    461  HA  THR A 198      30.533  53.828 -14.914  1.00  0.00           H
ATOM    462  HB  THR A 198      33.018  54.771 -13.548  1.00  0.00           H
ATOM    463 1HG2 THR A 198      31.357  55.432 -11.836  1.00  0.00           H
ATOM    464 2HG2 THR A 198      31.014  56.229 -13.390  1.00  0.00           H
ATOM    465 3HG2 THR A 198      30.042  54.830 -12.874  1.00  0.00           H
ATOM    466  HG1 THR A 198      32.354  53.309 -11.932  1.00  0.00           H
ATOM    467  N   ARG A 199      32.920  56.011 -15.806  1.00  0.00           N
ATOM    468  CA  ARG A 199      33.281  57.232 -16.514  1.00  0.00           C
ATOM    469  C   ARG A 199      32.465  58.437 -16.038  1.00  0.00           C
ATOM    470  O   ARG A 199      32.035  59.259 -16.842  1.00  0.00           O
ATOM    471  CB  ARG A 199      33.273  57.037 -18.039  1.00  0.00           C
ATOM    472  CG  ARG A 199      34.168  55.852 -18.427  1.00  0.00           C
ATOM    473  CD  ARG A 199      34.241  55.660 -19.946  1.00  0.00           C
ATOM    474  NE  ARG A 199      34.983  54.432 -20.274  1.00  0.00           N
ATOM    475  CZ  ARG A 199      34.517  53.185 -20.168  1.00  0.00           C
ATOM    476  NH1 ARG A 199      33.274  52.984 -19.729  1.00  0.00           N1+
ATOM    477  NH2 ARG A 199      35.282  52.142 -20.460  1.00  0.00           N
ATOM    478  H   ARG A 199      33.652  55.664 -15.202  1.00  0.00           H
ATOM    479  HA  ARG A 199      34.363  57.360 -16.490  1.00  0.00           H
ATOM    480 1HB  ARG A 199      32.255  56.840 -18.376  1.00  0.00           H
ATOM    481 2HB  ARG A 199      33.648  57.939 -18.523  1.00  0.00           H
ATOM    482 1HG  ARG A 199      35.179  56.023 -18.057  1.00  0.00           H
ATOM    483 2HG  ARG A 199      33.771  54.937 -17.987  1.00  0.00           H
ATOM    484 1HD  ARG A 199      33.233  55.583 -20.352  1.00  0.00           H
ATOM    485 2HD  ARG A 199      34.750  56.512 -20.397  1.00  0.00           H
ATOM    486  HE  ARG A 199      35.923  54.593 -20.606  1.00  0.00           H
ATOM    487 1HH1 ARG A 199      32.914  52.044 -19.645  1.00  0.00           H
ATOM    488 2HH1 ARG A 199      32.692  53.771 -19.480  1.00  0.00           H
ATOM    489 1HH2 ARG A 199      34.913  51.206 -20.373  1.00  0.00           H
ATOM    490 2HH2 ARG A 199      36.233  52.284 -20.768  1.00  0.00           H
ATOM    491  N   TYR A 200      32.360  58.599 -14.718  1.00  0.00           N
ATOM    492  CA  TYR A 200      32.104  59.912 -14.145  1.00  0.00           C
ATOM    493  C   TYR A 200      33.428  60.673 -14.244  1.00  0.00           C
ATOM    494  O   TYR A 200      34.476  60.092 -13.964  1.00  0.00           O
ATOM    495  CB  TYR A 200      31.682  59.800 -12.671  1.00  0.00           C
ATOM    496  CG  TYR A 200      30.539  58.853 -12.348  1.00  0.00           C
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ATOM    497  CD1 TYR A 200      29.485   58.626  -13.256  1.00  0.00          C
ATOM    498  CD2 TYR A 200      30.519   58.177  -11.112  1.00  0.00          C
ATOM    499  CE1 TYR A 200      28.457   57.717  -12.948  1.00  0.00          C
ATOM    500  CE2 TYR A 200      29.489   57.274  -10.801  1.00  0.00          C
ATOM    501  CZ  TYR A 200      28.460   57.023  -11.725  1.00  0.00          C
ATOM    502  OH  TYR A 200      27.480   56.116  -11.443  1.00  0.00          O
ATOM    503  H   TYR A 200      32.458   57.804  -14.102  1.00  0.00          H
ATOM    504  HA  TYR A 200      31.332   60.418  -14.724  1.00  0.00          H
ATOM    505  1HB TYR A 200      32.526   59.451  -12.076  1.00  0.00          H
ATOM    506  2HB TYR A 200      31.362   60.777  -12.308  1.00  0.00          H
ATOM    507  HD1 TYR A 200      29.461   59.152  -14.199  1.00  0.00          H
ATOM    508  HD2 TYR A 200      31.303   58.351  -10.390  1.00  0.00          H
ATOM    509  HE1 TYR A 200      27.657   57.548  -13.653  1.00  0.00          H
ATOM    510  HE2 TYR A 200      29.485   56.768   -9.847  1.00  0.00          H
ATOM    511  HH  TYR A 200      27.634   55.738  -10.574  1.00  0.00          H
ATOM    512  N   THR A 201      33.408   61.940  -14.648  1.00  0.00          N
ATOM    513  CA  THR A 201      34.606   62.659  -15.052  1.00  0.00          C
ATOM    514  C   THR A 201      35.003   63.733  -14.031  1.00  0.00          C
ATOM    515  O   THR A 201      35.990   64.437  -14.234  1.00  0.00          O
ATOM    516  CB  THR A 201      34.302   63.278  -16.426  1.00  0.00          C
ATOM    517  CG2 THR A 201      34.368   62.209  -17.523  1.00  0.00          C
ATOM    518  OG1 THR A 201      32.986   63.813  -16.420  1.00  0.00          O
ATOM    519  H   THR A 201      32.534   62.445  -14.683  1.00  0.00          H
ATOM    520  HA  THR A 201      35.426   61.954  -15.183  1.00  0.00          H
ATOM    521  HB  THR A 201      35.050   64.036  -16.657  1.00  0.00          H
ATOM    522  1HG2 THR A 201     34.150   62.665  -18.489  1.00  0.00          H
ATOM    523  2HG2 THR A 201     35.366   61.772  -17.545  1.00  0.00          H
ATOM    524  3HG2 THR A 201     33.634   61.430  -17.316  1.00  0.00          H
ATOM    525  HG1 THR A 201      32.793   64.200  -17.277  1.00  0.00          H
ATOM    526  N   ARG A 202      34.229   63.910  -12.958  1.00  0.00          N
ATOM    527  CA  ARG A 202      34.471   64.940  -11.963  1.00  0.00          C
ATOM    528  C   ARG A 202      33.552   64.651  -10.771  1.00  0.00          C
ATOM    529  O   ARG A 202      32.389   64.321  -11.000  1.00  0.00          O
ATOM    530  CB  ARG A 202      34.119   66.311  -12.571  1.00  0.00          C
ATOM    531  CG  ARG A 202      34.620   67.515  -11.763  1.00  0.00          C
ATOM    532  CD  ARG A 202      36.138   67.723  -11.893  1.00  0.00          C
ATOM    533  NE  ARG A 202      36.512   69.084  -11.473  1.00  0.00          N
ATOM    534  CZ  ARG A 202      37.710   69.473  -11.007  1.00  0.00          C
ATOM    535  NH1 ARG A 202      38.660   68.594  -10.708  1.00  0.00          N1+
ATOM    536  NH2 ARG A 202      37.955   70.770  -10.854  1.00  0.00          N
ATOM    537  H   ARG A 202      33.430   63.311  -12.808  1.00  0.00          H
ATOM    538  HA  ARG A 202      35.511   64.896  -11.638  1.00  0.00          H
ATOM    539  1HB ARG A 202      34.560   66.392  -13.564  1.00  0.00          H
ATOM    540  2HB ARG A 202      33.036   66.409  -12.645  1.00  0.00          H
ATOM    541  1HG ARG A 202      34.127   68.421  -12.116  1.00  0.00          H
ATOM    542  2HG ARG A 202      34.392   67.366  -10.707  1.00  0.00          H
ATOM    543  1HD ARG A 202      36.659   67.003  -11.261  1.00  0.00          H
ATOM    544  2HD ARG A 202      36.438   67.579  -12.931  1.00  0.00          H
ATOM    545  HE  ARG A 202      35.763   69.755  -11.563  1.00  0.00          H
ATOM    546  1HH1 ARG A 202     39.552   68.914  -10.359  1.00  0.00          H
ATOM    547  2HH1 ARG A 202     38.490   67.606  -10.830  1.00  0.00          H
ATOM    548  1HH2 ARG A 202     38.851   71.076  -10.504  1.00  0.00          H
ATOM    549  2HH2 ARG A 202     37.245   71.449  -11.087  1.00  0.00          H
ATOM    550  N   PRO A 203      34.011   64.763   -9.518  1.00  0.00          N
ATOM    551  CA  PRO A 203      33.125   64.663   -8.373  1.00  0.00          C
ATOM    552  C   PRO A 203      32.154   65.851   -8.359  1.00  0.00          C
ATOM    553  O   PRO A 203      32.542   66.990   -8.626  1.00  0.00          O
ATOM    554  CB  PRO A 203      34.037   64.649   -7.141  1.00  0.00          C
ATOM    555  CG  PRO A 203      35.308   65.348   -7.619  1.00  0.00          C
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ATOM    556  CD  PRO A 203      35.387  64.934  -9.086  1.00  0.00           C
ATOM    557  HA  PRO A 203      32.572  63.725  -8.421  1.00  0.00           H
ATOM    558 1HB  PRO A 203      33.554  65.186  -6.325  1.00  0.00           H
ATOM    559 2HB  PRO A 203      34.223  63.619  -6.838  1.00  0.00           H
ATOM    560 1HG  PRO A 203      35.201  66.425  -7.491  1.00  0.00           H
ATOM    561 2HG  PRO A 203      36.158  64.996  -7.036  1.00  0.00           H
ATOM    562 1HD  PRO A 203      35.925  63.993  -9.205  1.00  0.00           H
ATOM    563 2HD  PRO A 203      35.865  65.704  -9.692  1.00  0.00           H
ATOM    564  N   THR A 204      30.893  65.583  -8.036  1.00  0.00           N
ATOM    565  CA  THR A 204      29.847  66.584  -7.973  1.00  0.00           C
ATOM    566  C   THR A 204      30.030  67.465  -6.719  1.00  0.00           C
ATOM    567  O   THR A 204      30.884  67.169  -5.879  1.00  0.00           O
ATOM    568  CB  THR A 204      28.505  65.834  -7.951  1.00  0.00           C
ATOM    569  CG2 THR A 204      28.314  64.958  -9.196  1.00  0.00           C
ATOM    570  OG1 THR A 204      28.440  65.017  -6.796  1.00  0.00           O
ATOM    571  H   THR A 204      30.618  64.636  -7.816  1.00  0.00           H
ATOM    572  HA  THR A 204      29.873  67.195  -8.876  1.00  0.00           H
ATOM    573  HB  THR A 204      27.687  66.552  -7.892  1.00  0.00           H
ATOM    574 1HG2 THR A 204      27.353  64.447  -9.137  1.00  0.00           H
ATOM    575 2HG2 THR A 204      28.338  65.584 -10.088  1.00  0.00           H
ATOM    576 3HG2 THR A 204      29.114  64.220  -9.248  1.00  0.00           H
ATOM    577  HG1 THR A 204      27.602  64.549  -6.782  1.00  0.00           H
ATOM    578  N   PRO A 205      29.222  68.522  -6.515  1.00  0.00           N
ATOM    579  CA  PRO A 205      29.477  69.462  -5.430  1.00  0.00           C
ATOM    580  C   PRO A 205      29.371  68.813  -4.047  1.00  0.00           C
ATOM    581  O   PRO A 205      30.072  69.205  -3.116  1.00  0.00           O
ATOM    582  CB  PRO A 205      28.463  70.592  -5.610  1.00  0.00           C
ATOM    583  CG  PRO A 205      28.256  70.609  -7.124  1.00  0.00           C
ATOM    584  CD  PRO A 205      28.307  69.123  -7.479  1.00  0.00           C
ATOM    585  HA  PRO A 205      30.466  69.904  -5.557  1.00  0.00           H
ATOM    586 1HB  PRO A 205      27.552  70.354  -5.061  1.00  0.00           H
ATOM    587 2HB  PRO A 205      28.883  71.522  -5.230  1.00  0.00           H
ATOM    588 1HG  PRO A 205      27.294  71.066  -7.355  1.00  0.00           H
ATOM    589 2HG  PRO A 205      29.054  71.184  -7.594  1.00  0.00           H
ATOM    590 1HD  PRO A 205      28.688  68.968  -8.488  1.00  0.00           H
ATOM    591 2HD  PRO A 205      27.325  68.658  -7.387  1.00  0.00           H
ATOM    592  N   VAL A 206      28.512  67.802  -3.918  1.00  0.00           N
ATOM    593  CA  VAL A 206      28.405  67.041  -2.686  1.00  0.00           C
ATOM    594  C   VAL A 206      29.623  66.124  -2.570  1.00  0.00           C
ATOM    595  O   VAL A 206      30.285  66.101  -1.536  1.00  0.00           O
ATOM    596  CB  VAL A 206      27.049  66.310  -2.578  1.00  0.00           C
ATOM    597  CGI VAL A 206      26.705  65.407  -3.770  1.00  0.00           C
ATOM    598  CG2 VAL A 206      26.984  65.470  -1.296  1.00  0.00           C
ATOM    599  H   VAL A 206      27.913  67.547  -4.691  1.00  0.00           H
ATOM    600  HA  VAL A 206      28.250  67.723  -1.849  1.00  0.00           H
ATOM    601  HB  VAL A 206      26.252  67.040  -2.439  1.00  0.00           H
ATOM    602 1HG1 VAL A 206      25.736  64.937  -3.602  1.00  0.00           H
ATOM    603 2HG1 VAL A 206      26.667  66.004  -4.680  1.00  0.00           H
ATOM    604 3HG1 VAL A 206      27.469  64.636  -3.874  1.00  0.00           H
ATOM    605 1HG2 VAL A 206      26.020  64.963  -1.242  1.00  0.00           H
ATOM    606 2HG2 VAL A 206      27.783  64.728  -1.305  1.00  0.00           H
ATOM    607 3HG2 VAL A 206      27.102  66.119  -0.429  1.00  0.00           H
ATOM    608  N   GLN A 207      29.925  65.369  -3.627  1.00  0.00           N
ATOM    609  CA  GLN A 207      31.005  64.396  -3.629  1.00  0.00           C
ATOM    610  C   GLN A 207      32.336  65.058  -3.274  1.00  0.00           C
ATOM    611  O   GLN A 207      33.113  64.493  -2.509  1.00  0.00           O
ATOM    612  CB  GLN A 207      31.071  63.717  -4.998  1.00  0.00           C
ATOM    613  CG  GLN A 207      29.864  62.794  -5.211  1.00  0.00           C
ATOM    614  CD  GLN A 207      29.741  62.299  -6.644  1.00  0.00           C
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ATOM    615  NE2 GLN A 207      28.753   61.456   -6.924  1.00  0.00           N
ATOM    616  OE1 GLN A 207      30.535   62.663   -7.504  1.00  0.00           O
ATOM    617  H   GLN A 207      29.391   65.458   -4.480  1.00  0.00           H
ATOM    618  HA  GLN A 207      30.769   63.589   -2.936  1.00  0.00           H
ATOM    619  1HB GLN A 207      31.075   64.475   -5.781  1.00  0.00           H
ATOM    620  2HB GLN A 207      31.982   63.122   -5.065  1.00  0.00           H
ATOM    621  1HG GLN A 207      29.955   61.921   -4.565  1.00  0.00           H
ATOM    622  2HG GLN A 207      28.948   63.332   -4.967  1.00  0.00           H
ATOM    623  1HE2 GLN A 207     28.640   61.105   -7.864  1.00  0.00           H
ATOM    624  2HE2 GLN A 207     28.115   61.166   -6.197  1.00  0.00           H
ATOM    625  N   LYS A 208      32.591   66.247   -3.824  1.00  0.00           N
ATOM    626  CA  LYS A 208      33.777   67.041   -3.530  1.00  0.00           C
ATOM    627  C   LYS A 208      34.098   67.062   -2.029  1.00  0.00           C
ATOM    628  O   LYS A 208      35.270   67.063   -1.656  1.00  0.00           O
ATOM    629  CB  LYS A 208      33.562   68.481   -4.027  1.00  0.00           C
ATOM    630  CG  LYS A 208      33.764   68.660   -5.544  1.00  0.00           C
ATOM    631  CD  LYS A 208      35.226   68.945   -5.934  1.00  0.00           C
ATOM    632  CE  LYS A 208      35.670   70.374   -5.560  1.00  0.00           C
ATOM    633  NZ  LYS A 208      37.118   70.595   -5.742  1.00  0.00           N1+
ATOM    634  H   LYS A 208      31.942   66.647   -4.486  1.00  0.00           H
ATOM    635  HA  LYS A 208      34.629   66.637   -4.076  1.00  0.00           H
ATOM    636  1HB LYS A 208      32.544   68.796   -3.800  1.00  0.00           H
ATOM    637  2HB LYS A 208      34.268   69.147   -3.529  1.00  0.00           H
ATOM    638  1HG LYS A 208      33.457   67.751   -6.062  1.00  0.00           H
ATOM    639  2HG LYS A 208      33.161   69.498   -5.895  1.00  0.00           H
ATOM    640  1HD LYS A 208      35.884   68.245   -5.419  1.00  0.00           H
ATOM    641  2HD LYS A 208      35.345   68.829   -7.012  1.00  0.00           H
ATOM    642  1HE LYS A 208      35.144   71.094   -6.187  1.00  0.00           H
ATOM    643  2HE LYS A 208      35.435   70.566   -4.513  1.00  0.00           H
ATOM    644  1HZ LYS A 208      37.350   71.543   -5.483  1.00  0.00           H
ATOM    645  2HZ LYS A 208      37.633   69.951   -5.158  1.00  0.00           H
ATOM    646  3HZ LYS A 208      37.364   70.441   -6.709  1.00  0.00           H
ATOM    647  N   HIS A 209      33.066   67.136   -1.188  1.00  0.00           N
ATOM    648  CA  HIS A 209      33.197   67.389    0.238  1.00  0.00           C
ATOM    649  C   HIS A 209      32.878   66.119    1.022  1.00  0.00           C
ATOM    650  O   HIS A 209      33.548   65.808    2.002  1.00  0.00           O
ATOM    651  CB  HIS A 209      32.257   68.533    0.634  1.00  0.00           C
ATOM    652  CG  HIS A 209      32.538   69.805   -0.126  1.00  0.00           C
ATOM    653  CD2 HIS A 209      33.452   70.810    0.075  1.00  0.00           C
ATOM    654  ND1 HIS A 209      31.846   70.168   -1.277  1.00  0.00           N
ATOM    655  CE1 HIS A 209      32.354   71.328   -1.720  1.00  0.00           C
ATOM    656  NE2 HIS A 209      33.362   71.738   -0.953  1.00  0.00           N
ATOM    657  H   HIS A 209      32.124   67.013   -1.532  1.00  0.00           H
ATOM    658  HA  HIS A 209      34.207   67.738    0.454  1.00  0.00           H
ATOM    659  1HB HIS A 209      31.226   68.244    0.431  1.00  0.00           H
ATOM    660  2HB HIS A 209      32.371   68.746    1.697  1.00  0.00           H
ATOM    661  HD2 HIS A 209      34.100   70.786    0.939  1.00  0.00           H
ATOM    662  HD1 HIS A 209      31.103   69.579   -1.626  1.00  0.00           H
ATOM    663  HE1 HIS A 209      31.937   71.801   -2.597  1.00  0.00           H
ATOM    664  N   ALA A 210      31.858   65.374    0.601  1.00  0.00           N
ATOM    665  CA  ALA A 210      31.453   64.164    1.292  1.00  0.00           C
ATOM    666  C   ALA A 210      32.590   63.143    1.287  1.00  0.00           C
ATOM    667  O   ALA A 210      32.787   62.439    2.272  1.00  0.00           O
ATOM    668  CB  ALA A 210      30.194   63.585    0.643  1.00  0.00           C
ATOM    669  H   ALA A 210      31.341   65.645   -0.223  1.00  0.00           H
ATOM    670  HA  ALA A 210      31.148   64.410    2.309  1.00  0.00           H
ATOM    671  1HB ALA A 210      29.898   62.677    1.168  1.00  0.00           H
ATOM    672  2HB ALA A 210      29.388   64.316    0.698  1.00  0.00           H
ATOM    673  3HB ALA A 210      30.399   63.349   -0.402  1.00  0.00           H
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ATOM    674  N   ILE A 211     33.312  63.034   0.169  1.00  0.00           N
ATOM    675  CA  ILE A 211      34.407  62.086   0.060  1.00  0.00           C
ATOM    676  C   ILE A 211     35.436  62.326   1.181  1.00  0.00           C
ATOM    677  O   ILE A 211     35.715  61.398   1.940  1.00  0.00           O
ATOM    678  CB  ILE A 211      34.963  62.025  -1.381  1.00  0.00           C
ATOM    679  CG1 ILE A 211      33.864  61.511  -2.337  1.00  0.00           C
ATOM    680  CG2 ILE A 211      36.186  61.097  -1.442  1.00  0.00           C
ATOM    681  CD1 ILE A 211      34.223  61.629  -3.823  1.00  0.00           C
ATOM    682  H   ILE A 211     33.101  63.618  -0.627  1.00  0.00           H
ATOM    683  HA  ILE A 211      34.007  61.078  -0.052  1.00  0.00           H
ATOM    684  HB  ILE A 211      35.294  63.018  -1.686  1.00  0.00           H
ATOM    685 1HG1 ILE A 211      33.672  60.456  -2.137  1.00  0.00           H
ATOM    686 2HG1 ILE A 211      32.949  62.082  -2.182  1.00  0.00           H
ATOM    687 1HG2 ILE A 211      36.567  61.063  -2.462  1.00  0.00           H
ATOM    688 2HG2 ILE A 211      36.963  61.474  -0.777  1.00  0.00           H
ATOM    689 3HG2 ILE A 211      35.897  60.093  -1.129  1.00  0.00           H
ATOM    690 1HD1 ILE A 211      33.400  61.247  -4.427  1.00  0.00           H
ATOM    691 2HD1 ILE A 211      34.400  62.676  -4.072  1.00  0.00           H
ATOM    692 3HD1 ILE A 211      35.123  61.050  -4.027  1.00  0.00           H
ATOM    693  N   PRO A 212     36.004  63.532   1.332  1.00  0.00           N
ATOM    694  CA  PRO A 212      37.029  63.752   2.339  1.00  0.00           C
ATOM    695  C   PRO A 212     36.454  63.715   3.758  1.00  0.00           C
ATOM    696  O   PRO A 212     37.130  63.261   4.678  1.00  0.00           O
ATOM    697  CB  PRO A 212      37.694  65.092   2.012  1.00  0.00           C
ATOM    698  CG  PRO A 212      36.707  65.772   1.065  1.00  0.00           C
ATOM    699  CD  PRO A 212      36.033  64.602   0.355  1.00  0.00           C
ATOM    700  HA  PRO A 212      37.822  63.013   2.219  1.00  0.00           H
ATOM    701 1HB  PRO A 212      37.838  65.661   2.931  1.00  0.00           H
ATOM    702 2HB  PRO A 212      38.660  64.914   1.540  1.00  0.00           H
ATOM    703 IHG  PRO A 212      36.001  66.369   1.642  1.00  0.00           H
ATOM    704 2HG  PRO A 212      37.250  66.418  0.376  1.00  0.00           H
ATOM    705 IHD  PRO A 212      36.602  64.281  -0.518  1.00  0.00           H
ATOM    706 2HD  PRO A 212      35.015  64.848   0.055  1.00  0.00           H
ATOM    707  N   ILE A 213     35.212  64.165   3.955  1.00  0.00           N
ATOM    708  CA  ILE A 213      34.601  64.106   5.278  1.00  0.00           C
ATOM    709  C   ILE A 213     34.507  62.645   5.724  1.00  0.00           C
ATOM    710  O   ILE A 213     34.860  62.315   6.854  1.00  0.00           O
ATOM    711  CB  ILE A 213      33.225  64.800   5.302  1.00  0.00           C
ATOM    712  CGI ILE A 213      33.372  66.316   5.082  1.00  0.00           C
ATOM    713  CG2 ILE A 213      32.550  64.553   6.662  1.00  0.00           C
ATOM    714  CD1 ILE A 213      32.060  66.963   4.622  1.00  0.00           C
ATOM    715  H   ILE A 213     34.687  64.551  3.184  1.00  0.00           H
ATOM    716  HA  ILE A 213      35.170  64.726   5.970  1.00  0.00           H
ATOM    717  HB  ILE A 213      32.595  64.386   4.515  1.00  0.00           H
ATOM    718 1HG1 ILE A 213      33.675  66.791   6.015  1.00  0.00           H
ATOM    719 2HG1 ILE A 213      34.127  66.502   4.319  1.00  0.00           H
ATOM    720 1HG2 ILE A 213      31.577  65.043   6.679  1.00  0.00           H
ATOM    721 2HG2 ILE A 213      32.419  63.481   6.814  1.00  0.00           H
ATOM    722 3HG2 ILE A 213      33.176  64.958   7.457  1.00  0.00           H
ATOM    723 1HD1 ILE A 213      32.213  68.033   4.480  1.00  0.00           H
ATOM    724 2HD1 ILE A 213      31.743  66.514   3.681  1.00  0.00           H
ATOM    725 3HD1 ILE A 213      31.291  66.804   5.378  1.00  0.00           H
ATOM    726  N   ILE A 214     34.020  61.771   4.844  1.00  0.00           N
ATOM    727  CA  ILE A 214      33.851  60.368   5.181  1.00  0.00           C
ATOM    728  C   ILE A 214     35.234  59.729   5.325  1.00  0.00           C
ATOM    729  O   ILE A 214     35.434  58.791   6.103  1.00  0.00           O
ATOM    730  CB  ILE A 214      32.978  59.682   4.111  1.00  0.00           C
ATOM    731  CG1 ILE A 214      31.559  60.283   4.157  1.00  0.00           C
ATOM    732  CG2 ILE A 214      32.914  58.160   4.318  1.00  0.00           C
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ATOM    733  CD1 ILE A 214      30.701  59.905   2.944  1.00  0.00           C
ATOM    734  H   ILE A 214      33.759  62.079   3.918  1.00  0.00           H
ATOM    735  HA  ILE A 214      33.245  60.281   6.083  1.00  0.00           H
ATOM    736  HB  ILE A 214      33.432  59.816   3.130  1.00  0.00           H
ATOM    737 1HG1 ILE A 214      31.041  59.927   5.047  1.00  0.00           H
ATOM    738 2HG1 ILE A 214      31.625  61.370   4.185  1.00  0.00           H
ATOM    739 1HG2 ILE A 214      32.289  57.713   3.545  1.00  0.00           H
ATOM    740 2HG2 ILE A 214      33.919  57.742   4.259  1.00  0.00           H
ATOM    741 3HG2 ILE A 214      32.489  57.943   5.298  1.00  0.00           H
ATOM    742 1HD1 ILE A 214      29.715  60.361   3.040  1.00  0.00           H
ATOM    743 2HD1 ILE A 214      31.179  60.265   2.033  1.00  0.00           H
ATOM    744 3HD1 ILE A 214      30.596  58.822   2.896  1.00  0.00           H
ATOM    745  N   LYS A 215      36.198  60.215   4.544  1.00  0.00           N
ATOM    746  CA  LYS A 215      37.553  59.729   4.629  1.00  0.00           C
ATOM    747  C   LYS A 215      38.141  60.049   6.007  1.00  0.00           C
ATOM    748  O   LYS A 215      38.822  59.206   6.602  1.00  0.00           O
ATOM    749  CB  LYS A 215      38.394  60.304   3.483  1.00  0.00           C
ATOM    750  CG  LYS A 215      39.829  59.776   3.465  1.00  0.00           C
ATOM    751  CD  LYS A 215      39.908  58.273   3.177  1.00  0.00           C
ATOM    752  CE  LYS A 215      41.270  57.754   3.628  1.00  0.00           C
ATOM    753  NZ  LYS A 215      41.382  56.304   3.400  1.00  0.00           N1+
ATOM    754  H   LYS A 215      35.988  60.940   3.874  1.00  0.00           H
ATOM    755  HA  LYS A 215      37.573  58.664   4.396  1.00  0.00           H
ATOM    756 1HB  LYS A 215      37.936  60.043   2.529  1.00  0.00           H
ATOM    757 2HB  LYS A 215      38.444  61.389   3.577  1.00  0.00           H
ATOM    758 1HG  LYS A 215      40.397  60.292   2.691  1.00  0.00           H
ATOM    759 2HG  LYS A 215      40.294  59.953   4.435  1.00  0.00           H
ATOM    760 1HD  LYS A 215      39.118  57.756   3.723  1.00  0.00           H
ATOM    761 2HD  LYS A 215      39.783  58.100   2.108  1.00  0.00           H
ATOM    762 1HE  LYS A 215      42.056  58.258   3.065  1.00  0.00           H
ATOM    763 2HE  LYS A 215      41.401  57.952   4.691  1.00  0.00           H
ATOM    764 1HZ  LYS A 215      42.290  55.984   3.705  1.00  0.00           H
ATOM    765 2HZ  LYS A 215      40.663  55.824   3.923  1.00  0.00           H
ATOM    766 3HZ  LYS A 215      41.270  56.107   2.416  1.00  0.00           H
ATOM    767  N   GLU A 216      37.876  61.252   6.515  1.00  0.00           N
ATOM    768  CA  GLU A 216      38.435  61.758   7.755  1.00  0.00           C
ATOM    769  C   GLU A 216      37.367  61.890   8.839  1.00  0.00           C
ATOM    770  O   GLU A 216      37.433  62.761   9.702  1.00  0.00           O
ATOM    771  CB  GLU A 216      39.290  63.007   7.501  1.00  0.00           C
ATOM    772  CG  GLU A 216      40.502  62.681   6.602  1.00  0.00           C
ATOM    773  CD  GLU A 216      41.312  61.512  61.515  7.148  1.00  0.00           C
ATOM    774  OE1 GLU A 216      41.524  61.472   8.379  1.00  0.00           O
ATOM    775  OE2 GLU A 216      41.550  60.537   6.408  1.00  0.00           Ol-
ATOM    776  H   GLU A 216      37.250  61.878   6.029  1.00  0.00           H
ATOM    777  HA  GLU A 216      39.327  61.187   8.012  1.00  0.00           H
ATOM    778 1HB  GLU A 216      38.685  63.767   7.007  1.00  0.00           H
ATOM    779 2HB  GLU A 216      39.657  63.396   8.451  1.00  0.00           H
ATOM    780 1HG  GLU A 216      40.154  62.417   5.603  1.00  0.00           H
ATOM    781 2HG  GLU A 216      41.155  63.551  6.541  1.00  0.00           H
ATOM    782  N   LYS A 217      36.498  60.878   8.884  1.00  0.00           N
ATOM    783  CA  LYS A 217      36.071  60.255  10.127  1.00  0.00           C
ATOM    784  C   LYS A 217      35.284  61.217  11.024  1.00  0.00           C
ATOM    785  O   LYS A 217      35.485  61.232  12.237  1.00  0.00           O
ATOM    786  CB  LYS A 217      37.304  59.673  10.855  1.00  0.00           C
ATOM    787  CG  LYS A 217      38.153  58.725   9.981  1.00  0.00           C
ATOM    788  CD  LYS A 217      39.587  58.599  10.527  1.00  0.00           C
ATOM    789  CE  LYS A 217      40.573  58.009   9.502  1.00  0.00           C
ATOM    790  NZ  LYS A 217      40.866  58.949   8.400  1.00  0.00           N1+
ATOM    791  H   LYS A 217      36.105  60.511  8.029  1.00  0.00           H
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ATOM    792  HA  LYS A 217      35.499  59.354   9.905  1.00  0.00           H
ATOM    793 1HB  LYS A 217      37.954  60.486  11.177  1.00  0.00           H
ATOM    794 2HB  LYS A 217      36.977  59.104  11.726  1.00  0.00           H
ATOM    795 1HG  LYS A 217      37.697  57.735   9.969  1.00  0.00           H
ATOM    796 2HG  LYS A 217      38.202  59.114   8.964  1.00  0.00           H
ATOM    797 1HD  LYS A 217      39.956  59.584  10.812  1.00  0.00           H
ATOM    798 2HD  LYS A 217      39.588  57.945  11.400  1.00  0.00           H
ATOM    799 1HE  LYS A 217      41.514  57.768   9.998  1.00  0.00           H
ATOM    800 2HE  LYS A 217      40.149  57.103   9.068  1.00  0.00           H
ATOM    801 1HZ  LYS A 217      41.514  58.521   7.755  1.00  0.00           H
ATOM    802 2HZ  LYS A 217      40.010  59.177   7.915  1.00  0.00           H
ATOM    803 3HZ  LYS A 217      41.273  59.793   8.776  1.00  0.00           H
ATOM    804  N   ARG A 218      34.359  61.971  10.435  1.00  0.00           N
ATOM    805  CA  ARG A 218      33.481  62.886  11.147  1.00  0.00           C
ATOM    806  C   ARG A 218      32.060  62.589  10.684  1.00  0.00           C
ATOM    807  O   ARG A 218      31.800  62.611  9.482  1.00  0.00           O
ATOM    808  CB  ARG A 218      33.851  64.331  10.795  1.00  0.00           C
ATOM    809  CG  ARG A 218      35.202  64.771  11.381  1.00  0.00           C
ATOM    810  CD  ARG A 218      35.125  65.172  12.864  1.00  0.00           C
ATOM    811  NE  ARG A 218      34.131  66.227  13.125  1.00  0.00           N
ATOM    812  CZ  ARG A 218      34.188  67.503  12.729  1.00  0.00           C
ATOM    813  NH1 ARG A 218      35.228  67.927  12.011  1.00  0.00           N1+
ATOM    814  NH2 ARG A 218      33.200  68.345  12.995  1.00  0.00           N
ATOM    815  H   ARG A 218      34.235  61.927   9.434  1.00  0.00           H
ATOM    816  HA  ARG A 218      33.565  62.710  12.220  1.00  0.00           H
ATOM    817 1HB  ARG A 218      33.912  64.438   9.712  1.00  0.00           H
ATOM    818 2HB  ARG A 218      33.089  65.007  11.184  1.00  0.00           H
ATOM    819 1HG  ARG A 218      35.917  63.953  11.301  1.00  0.00           H
ATOM    820 2HG  ARG A 218      35.574  65.634  10.829  1.00  0.00           H
ATOM    821 1HD  ARG A 218      34.850  64.303  13.462  1.00  0.00           H
ATOM    822 2HD  ARG A 218      36.096  65.544  13.191  1.00  0.00           H
ATOM    823  HE  ARG A 218      33.342  65.901  13.665  1.00  0.00           H
ATOM    824 1HH1 ARG A 218      35.274  68.890  11.709  1.00  0.00           H
ATOM    825 2HH1 ARG A 218      35.969  67.285  11.768  1.00  0.00           H
ATOM    826 1HH2 ARG A 218      33.258  69.306  12.688  1.00  0.00           H
ATOM    827 2HH2 ARG A 218      32.388  68.027  13.505  1.00  0.00           H
ATOM    828  N   ASP A 219      31.163  62.301  11.628  1.00  0.00           N
ATOM    829  CA  ASP A 219      29.793  61.909  11.335  1.00  0.00           C
ATOM    830  C   ASP A 219      29.087  63.039  10.577  1.00  0.00           C
ATOM    831  O   ASP A 219      29.419  64.217  10.735  1.00  0.00           O
ATOM    832  CB  ASP A 219      29.075  61.415  12.608  1.00  0.00           C
ATOM    833  CG  ASP A 219      29.380  59.951  12.922  1.00  0.00           C
ATOM    834  OD1 ASP A 219      30.307  59.393  12.299  1.00  0.00           O
ATOM    835  OD2 ASP A 219      28.643  59.327  13.715  1.00  0.00           Ol-
ATOM    836  H   ASP A 219      31.423  62.350  12.603  1.00  0.00           H
ATOM    837  HA  ASP A 219      29.789  60.930  10.855  1.00  0.00           H
ATOM    838 1HB  ASP A 219      29.393  62.014  13.461  1.00  0.00           H
ATOM    839 2HB  ASP A 219      27.997  61.512  12.478  1.00  0.00           H
ATOM    840  N   LEU A 220      28.168  62.679   9.682  1.00  0.00           N
ATOM    841  CA  LEU A 220      27.842  63.509   8.531  1.00  0.00           C
ATOM    842  C   LEU A 220      26.334  63.543   8.301  1.00  0.00           C
ATOM    843  O   LEU A 220      25.679  62.502   8.282  1.00  0.00           O
ATOM    844  CB  LEU A 220      28.568  62.932   7.303  1.00  0.00           C
ATOM    845  CG  LEU A 220      28.181  63.556   5.948  1.00  0.00           C
ATOM    846  CD1 LEU A 220      28.521  65.049   5.869  1.00  0.00           C
ATOM    847  CD2 LEU A 220      28.932  62.824   4.830  1.00  0.00           C
ATOM    848  H   LEU A 220      27.672  61.806   9.791  1.00  0.00           H
ATOM    849  HA  LEU A 220      28.218  64.519   8.693  1.00  0.00           H
ATOM    850 1HB  LEU A 220      29.643  63.080   7.413  1.00  0.00           H
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ATOM    851 2HB  LEU A 220      28.355  61.866   7.222  1.00  0.00           H
ATOM    852  HG  LEU A 220      27.109  63.440   5.787  1.00  0.00           H
ATOM    853 1HD1 LEU A 220      28.228  65.438   4.894  1.00  0.00           H
ATOM    854 2HD1 LEU A 220      27.984  65.586   6.651  1.00  0.00           H
ATOM    855 3HD1 LEU A 220      29.594  65.185   6.006  1.00  0.00           H
ATOM    856 1HD2 LEU A 220      28.664  63.258   3.867  1.00  0.00           H
ATOM    857 2HD2 LEU A 220      30.006  62.923   4.988  1.00  0.00           H
ATOM    858 3HD2 LEU A 220      28.660  61.768   4.841  1.00  0.00           H
ATOM    859  N   MET A 221      25.811  64.741   8.040  1.00  0.00           N
ATOM    860  CA  MET A 221      24.512  64.949   7.428  1.00  0.00           C
ATOM    861  C   MET A 221      24.793  65.579   6.068  1.00  0.00           C
ATOM    862  O   MET A 221      25.418  66.636   6.016  1.00  0.00           O
ATOM    863  CB  MET A 221      23.701  65.911  8.302  1.00  0.00           C
ATOM    864  CG  MET A 221      22.294  66.179   7.764  1.00  0.00           C
ATOM    865  SD  MET A 221      21.200  64.741   7.836  1.00  0.00           S
ATOM    866  CE  MET A 221      20.778  64.575   6.086  1.00  0.00           C
ATOM    867  H   MET A 221      26.327  65.578   8.272  1.00  0.00           H
ATOM    868  HA  MET A 221      24.013  63.988   7.298  1.00  0.00           H
ATOM    869 1HB  MET A 221      23.594  65.492   9.303  1.00  0.00           H
ATOM    870 2HB  MET A 221      24.216  66.870   8.363  1.00  0.00           H
ATOM    871 1HG  MET A 221      21.826  66.971   8.348  1.00  0.00           H
ATOM    872 2HG  MET A 221      22.356  66.486   6.720  1.00  0.00           H
ATOM    873 1HE  MET A 221      20.104  63.728   5.953  1.00  0.00           H
ATOM    874 2HE  MET A 221      20.288  65.486   5.741  1.00  0.00           H
ATOM    875 3HE  MET A 221      21.686  64.410   5.506  1.00  0.00           H
ATOM    876  N   ALA A 222      24.347  64.959   4.980  1.00  0.00           N
ATOM    877  CA  ALA A 222      24.584  65.429   3.627  1.00  0.00           C
ATOM    878  C   ALA A 222      23.273  65.385   2.846  1.00  0.00           C
ATOM    879  O   ALA A 222      22.987  64.419   2.143  1.00  0.00           O
ATOM    880  CB  ALA A 222      25.652  64.546   2.983  1.00  0.00           C
ATOM    881  H   ALA A 222      23.809  64.108   5.068  1.00  0.00           H
ATOM    882  HA  ALA A 222      24.990  66.440   3.659  1.00  0.00           H
ATOM    883 1HB  ALA A 222      25.841  64.887   1.965  1.00  0.00           H
ATOM    884 2HB  ALA A 222      26.573  64.607   3.563  1.00  0.00           H
ATOM    885 3HB  ALA A 222      25.306  63.513   2.960  1.00  0.00           H
ATOM    886  N   CYS A 223      22.484  66.452   2.939  1.00  0.00           N
ATOM    887  CA  CYS A 223      21.190  66.511   2.278  1.00  0.00           C
ATOM    888  C   CYS A 223      21.400  66.872   0.806  1.00  0.00           C
ATOM    889  O   CYS A 223      22.098  67.839   0.503  1.00  0.00           O
ATOM    890  CB  CYS A 223      20.293  67.531  2.991  1.00  0.00           C
ATOM    891  SG  CYS A 223      18.814  67.867   2.002  1.00  0.00           S
ATOM    892  H   CYS A 223      22.778  67.253   3.479  1.00  0.00           H
ATOM    893  HA  CYS A 223      20.680  65.555   2.392  1.00  0.00           H
ATOM    894 1HB  CYS A 223      19.991  67.136   3.960  1.00  0.00           H
ATOM    895 2HB  CYS A 223      20.843  68.462   3.135  1.00  0.00           H
ATOM    896  HG  CYS A 223      18.181  68.600   2.524  1.00  0.00           H
ATOM    897  N   ALA A 224      20.787  66.149  -0.130  1.00  0.00           N
ATOM    898  CA  ALA A 224      20.885  66.493  -1.538  1.00  0.00           C
ATOM    899  C   ALA A 224      19.762  65.830  -2.329  1.00  0.00           C
ATOM    900  O   ALA A 224      19.564  64.622  -2.231  1.00  0.00           O
ATOM    901  CB  ALA A 224      22.248  66.060  -2.090  1.00  0.00           C
ATOM    902  H   ALA A 224      20.239  65.343   0.134  1.00  0.00           H
ATOM    903  HA  ALA A 224      20.842  67.576  -1.652  1.00  0.00           H
ATOM    904 1HB  ALA A 224      22.313  66.322  -3.146  1.00  0.00           H
ATOM    905 2HB  ALA A 224      23.041  66.568  -1.541  1.00  0.00           H
ATOM    906 3HB  ALA A 224      22.361  64.982  -1.976  1.00  0.00           H
ATOM    907  N   GLN A 225      19.052  66.602  -3.148  1.00  0.00           N
ATOM    908  CA  GLN A 225      18.011  66.070  -4.016  1.00  0.00           C
ATOM    909  C   GLN A 225      18.551  64.940  -4.907  1.00  0.00           C
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ATOM    910  O   GLN A 225      19.741  64.912  -5.232  1.00  0.00           O
ATOM    911  CB  GLN A 225      17.413  67.202  -4.863  1.00  0.00           C
ATOM    912  CG  GLN A 225      18.470  68.003  -5.638  1.00  0.00           C
ATOM    913  CD  GLN A 225      17.818  68.910  -6.670  1.00  0.00           C
ATOM    914  NE2 GLN A 225      17.664  70.190  -6.358  1.00  0.00           N
ATOM    915  OE1 GLN A 225      17.449  68.463  -7.751  1.00  0.00           O
ATOM    916  H   GLN A 225      19.227  67.596  -3.183  1.00  0.00           H
ATOM    917  HA  GLN A 225      17.172  65.728  -3.410  1.00  0.00           H
ATOM    918  1HB GLN A 225      16.719  66.782  -5.592  1.00  0.00           H
ATOM    919  2HB GLN A 225      16.881  67.899  -4.216  1.00  0.00           H
ATOM    920  1HG GLN A 225      19.042  68.618  -4.943  1.00  0.00           H
ATOM    921  2HG GLN A 225      19.142  67.316  -6.152  1.00  0.00           H
ATOM    922  1HE2 GLN A 225      17.236  70.823  -7.018  1.00  0.00           H
ATOM    923  2HE2 GLN A 225      17.976  70.532  -5.460  1.00  0.00           H
ATOM    924  N   THR A 226      17.683  64.025  -5.352  1.00  0.00           N
ATOM    925  CA  THR A 226      18.044  63.049  -6.365  1.00  0.00           C
ATOM    926  C   THR A 226      18.554  63.810  -7.602  1.00  0.00           C
ATOM    927  O   THR A 226      17.775  64.430  -8.323  1.00  0.00           O
ATOM    928  CB  THR A 226      16.816  62.179  -6.698  1.00  0.00           C
ATOM    929  CG2 THR A 226      17.227  60.752  -7.064  1.00  0.00           C
ATOM    930  OG1 THR A 226      15.894  62.136  -5.621  1.00  0.00           O
ATOM    931  H   THR A 226      16.743  63.999  -4.982  1.00  0.00           H
ATOM    932  HA  THR A 226      18.802  62.374  -5.967  1.00  0.00           H
ATOM    933  HB  THR A 226      16.258  62.636  -7.515  1.00  0.00           H
ATOM    934  1HG2 THR A 226      16.337  60.165  -7.293  1.00  0.00           H
ATOM    935  2HG2 THR A 226      17.881  60.774  -7.935  1.00  0.00           H
ATOM    936  3HG2 THR A 226      17.755  60.299  -6.225  1.00  0.00           H
ATOM    937  HG1 THR A 226      15.144  61.587  -5.863  1.00  0.00           H
ATOM    938  N   GLY A 227      19.865  63.807  -7.822  1.00  0.00           N
ATOM    939  CA  GLY A 227      20.512  64.935  -8.462  1.00  0.00           C
ATOM    940  C   GLY A 227      22.008  64.645  -8.481  1.00  0.00           C
ATOM    941  O   GLY A 227      22.442  63.739  -9.200  1.00  0.00           O
ATOM    942  H   GLY A 227      20.423  63.013  -7.542  1.00  0.00           H
ATOM    943  1HA  GLY A 227      20.130  65.045  -9.476  1.00  0.00           H
ATOM    944  2HA  GLY A 227      20.305  65.843  -7.895  1.00  0.00           H
ATOM    945  N   SER A 228      22.780  65.323  -7.633  1.00  0.00           N
ATOM    946  CA  SER A 228      24.234  65.300  -7.633  1.00  0.00           C
ATOM    947  C   SER A 228      24.863  63.984  -7.130  1.00  0.00           C
ATOM    948  O   SER A 228      25.941  64.007  -6.538  1.00  0.00           O
ATOM    949  CB  SER A 228      24.722  66.472  -6.771  1.00  0.00           C
ATOM    950  OG  SER A 228      24.226  67.710  -7.238  1.00  0.00           O
ATOM    951  H   SER A 228      22.360  65.907  -6.924  1.00  0.00           H
ATOM    952  HA  SER A 228      24.602  65.502  -8.639  1.00  0.00           H
ATOM    953  1HB  SER A 228      24.383  66.334  -5.744  1.00  0.00           H
ATOM    954  2HB  SER A 228      25.811  66.511  -6.792  1.00  0.00           H
ATOM    955  HG  SER A 228      24.551  68.418  -6.677  1.00  0.00           H
ATOM    956  N   GLY A 229      24.254  62.826  -7.387  1.00  0.00           N
ATOM    957  CA  GLY A 229      24.921  61.541  -7.240  1.00  0.00           C
ATOM    958  C   GLY A 229      25.317  61.222  -5.796  1.00  0.00           C
ATOM    959  O   GLY A 229      26.332  60.560  -5.569  1.00  0.00           O
ATOM    960  H   GLY A 229      23.293  62.819  -7.697  1.00  0.00           H
ATOM    961  1HA  GLY A 229      24.257  60.746  -7.580  1.00  0.00           H
ATOM    962  2HA  GLY A 229      25.832  61.533  -7.839  1.00  0.00           H
ATOM    963  N   LYS A 230      24.502  61.647  -4.825  1.00  0.00           N
ATOM    964  CA  LYS A 230      24.684  61.288  -3.423  1.00  0.00           C
ATOM    965  C   LYS A 230      24.821  59.772  -3.269  1.00  0.00           C
ATOM    966  O   LYS A 230      25.666  59.290  -2.522  1.00  0.00           O
ATOM    967  CB  LYS A 230      23.530  61.831  -2.571  1.00  0.00           C
ATOM    968  CG  LYS A 230      22.151  61.274  -2.955  1.00  0.00           C
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ATOM    969  CD  LYS A 230      21.072  61.917  -2.082  1.00  0.00           C
ATOM    970  CE  LYS A 230      19.661  61.665  -2.631  1.00  0.00           C
ATOM    971  NZ  LYS A 230      19.369  60.230  -2.811  1.00  0.00           N1+
ATOM    972  H   LYS A 230      23.718  62.243  -5.049  1.00  0.00           H
ATOM    973  HA  LYS A 230      25.549  61.817  -3.022  1.00  0.00           H
ATOM    974 IHB  LYS A 230      23.699  61.575  -1.525  1.00  0.00           H
ATOM    975 2HB  LYS A 230      23.479  62.915  -2.676  1.00  0.00           H
ATOM    976 1HG  LYS A 230      21.947  61.498  -4.003  1.00  0.00           H
ATOM    977 2HG  LYS A 230      22.139  60.195  -2.806  1.00  0.00           H
ATOM    978 1HD  LYS A 230      21.125  61.503  -1.076  1.00  0.00           H
ATOM    979 2HD  LYS A 230      21.233  62.994  -2.040  1.00  0.00           H
ATOM    980 1HE  LYS A 230      18.924  62.071  -1.939  1.00  0.00           H
ATOM    981 2HE  LYS A 230      19.555  62.151  -3.601  1.00  0.00           H
ATOM    982 1HZ  LYS A 230      18.432  60.120  -3.172  1.00  0.00           H
ATOM    983 2HZ  LYS A 230      20.030  59.830  -3.462  1.00  0.00           H
ATOM    984 3HZ  LYS A 230      19.444  59.757  -1.922  1.00  0.00           H
ATOM    985  N   THR A 231      24.011  59.037  -4.026  1.00  0.00           N
ATOM    986  CA  THR A 231      23.815  57.602  -3.941  1.00  0.00           C
ATOM    987  C   THR A 231      25.078  56.820  -4.348  1.00  0.00           C
ATOM    988  O   THR A 231      25.094  55.592  -4.295  1.00  0.00           O
ATOM    989  CB  THR A 231      22.590  57.314  -4.830  1.00  0.00           C
ATOM    990  CG2 THR A 231      22.007  55.908  -4.678  1.00  0.00           C
ATOM    991  OG1 THR A 231      21.578  58.256  -4.495  1.00  0.00           O
ATOM    992  H   THR A 231      23.455  59.478  -4.745  1.00  0.00           H
ATOM    993  HA  THR A 231      23.492  57.337  -2.934  1.00  0.00           H
ATOM    994  HB  THR A 231      22.863  57.440  -5.878  1.00  0.00           H
ATOM    995 1HG2 THR A 231      21.149  55.796  -5.341  1.00  0.00           H
ATOM    996 2HG2 THR A 231      22.766  55.170  -4.938  1.00  0.00           H
ATOM    997 3HG2 THR A 231      21.690  55.756  -3.647  1.00  0.00           H
ATOM    998  HG1 THR A 231      20.801  58.098  -5.037  1.00  0.00           H
ATOM    999  N   ALA A 232      26.140  57.513  -4.773  1.00  0.00           N
ATOM   1000  CA  ALA A 232      27.437  56.917  -5.048  1.00  0.00           C
ATOM   1001  C   ALA A 232      28.540  57.676  -4.305  1.00  0.00           C
ATOM   1002  O   ALA A 232      29.715  57.322  -4.398  1.00  0.00           O
ATOM   1003  CB  ALA A 232      27.693  56.951  -6.558  1.00  0.00           C
ATOM   1004  H   ALA A 232      26.066  58.510  -4.920  1.00  0.00           H
ATOM   1005  HA  ALA A 232      27.430  55.871  -4.742  1.00  0.00           H
ATOM   1006 IHB  ALA A 232      28.664  56.505  -6.772  1.00  0.00           H
ATOM   1007 2HB  ALA A 232      26.914  56.387  -7.071  1.00  0.00           H
ATOM   1008 3HB  ALA A 232      27.682  57.983  -6.906  1.00  0.00           H
ATOM   1009  N   ALA A 233      28.185  58.748  -3.597  1.00  0.00           N
ATOM   1010  CA  ALA A 233      29.153  59.681  -3.050  1.00  0.00           C
ATOM   1011  C   ALA A 233      29.873  59.069  -1.858  1.00  0.00           C
ATOM   1012  O   ALA A 233      31.019  59.410  -1.577  1.00  0.00           O
ATOM   1013  CB  ALA A 233      28.451  60.972  -2.623  1.00  0.00           C
ATOM   1014  H   ALA A 233      27.208  58.938  -3.424  1.00  0.00           H
ATOM   1015  HA  ALA A 233      29.874  59.952  -3.821  1.00  0.00           H
ATOM   1016 IHB  ALA A 233      29.184  61.667  -2.213  1.00  0.00           H
ATOM   1017 2HB  ALA A 233      27.966  61.425  -3.488  1.00  0.00           H
ATOM   1018 3HB  ALA A 233      27.701  60.746  -1.865  1.00  0.00           H
ATOM   1019  N   PHE A 234      29.174  58.196  -1.140  1.00  0.00           N
ATOM   1020  CA  PHE A 234      29.685  57.561   0.056  1.00  0.00           C
ATOM   1021  C   PHE A 234      30.371  56.244  -0.297  1.00  0.00           C
ATOM   1022  O   PHE A 234      31.084  55.687   0.529  1.00  0.00           O
ATOM   1023  CB  PHE A 234      28.536  57.341   1.043  1.00  0.00           C
ATOM   1024  CG  PHE A 234      27.297  56.711   0.438  1.00  0.00           C
ATOM   1025  CD1 PHE A 234      27.232  55.323   0.213  1.00  0.00           C
ATOM   1026  CD2 PHE A 234      26.188  57.508   0.091  1.00  0.00           C
ATOM   1027  CE1 PHE A 234      26.077  54.743  -0.336  1.00  0.00           C
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ATOM   1028  CE2 PHE A 234      25.027  56.929  -0.443  1.00  0.00           C
ATOM   1029  CZ  PHE A 234      24.971  55.545  -0.662  1.00  0.00           C
ATOM   1030  H   PHE A 234      28.236  57.947  -1.422  1.00  0.00           H
ATOM   1031  HA  PHE A 234      30.371  58.239   0.564  1.00  0.00           H
ATOM   1032  1HB PHE A 234      28.867  56.681   1.845  1.00  0.00           H
ATOM   1033  2HB PHE A 234      28.230  58.299   1.465  1.00  0.00           H
ATOM   1034  HD1 PHE A 234      28.076  54.696   0.462  1.00  0.00           H
ATOM   1035  HD2 PHE A 234      26.226  58.578   0.235  1.00  0.00           H
ATOM   1036  HE1 PHE A 234      26.039  53.677  -0.509  1.00  0.00           H
ATOM   1037  HE2 PHE A 234      24.177  57.549  -0.685  1.00  0.00           H
ATOM   1038  HZ  PHE A 234      24.082  55.095  -1.079  1.00  0.00           H
ATOM   1039  N   LEU A 235      30.157  55.721  -1.504  1.00  0.00           N
ATOM   1040  CA  LEU A 235      30.708  54.426  -1.867  1.00  0.00           C
ATOM   1041  C   LEU A 235      32.224  54.529  -2.000  1.00  0.00           C
ATOM   1042  O   LEU A 235      32.951  53.752  -1.388  1.00  0.00           O
ATOM   1043  CB  LEU A 235      30.069  53.888  -3.154  1.00  0.00           C
ATOM   1044  CG  LEU A 235      28.600  53.471  -2.969  1.00  0.00           C
ATOM   1045  CD1 LEU A 235      28.038  53.022  -4.320  1.00  0.00           C
ATOM   1046  CD2 LEU A 235      28.461  52.313  -1.969  1.00  0.00           C
ATOM   1047  H   LEU A 235      29.604  56.225  -2.183  1.00  0.00           H
ATOM   1048  HA  LEU A 235      30.405  53.682  -1.130  1.00  0.00           H
ATOM   1049  1HB LEU A 235      30.099  54.658  -3.924  1.00  0.00           H
ATOM   1050  2HB LEU A 235      30.620  53.012  -3.495  1.00  0.00           H
ATOM   1051  HG  LEU A 235      28.026  54.319  -2.595  1.00  0.00           H
ATOM   1052  1HD1 LEU A 235     26.997  52.724  -4.200  1.00  0.00           H
ATOM   1053  2HD1 LEU A 235     28.101  53.845  -5.032  1.00  0.00           H
ATOM   1054  3HD1 LEU A 235     28.617  52.176  -4.692  1.00  0.00           H
ATOM   1055  1HD2 LEU A 235     27.409  52.047  -1.865  1.00  0.00           H
ATOM   1056  2HD2 LEU A 235     29.019  51.450  -2.332  1.00  0.00           H
ATOM   1057  3HD2 LEU A 235     28.855  52.619  -1.000  1.00  0.00           H
ATOM   1058  N   LEU A 236      32.696  55.466  -2.821  1.00  0.00           N
ATOM   1059  CA  LEU A 236      34.120  55.663  -3.048  1.00  0.00           C
ATOM   1060  C   LEU A 236      34.903  55.781  -1.728  1.00  0.00           C
ATOM   1061  O   LEU A 236      35.898  55.076  -1.556  1.00  0.00           O
ATOM   1062  CB  LEU A 236      34.376  56.841  -4.002  1.00  0.00           C
ATOM   1063  CG  LEU A 236      33.635  56.740  -5.348  1.00  0.00           C
ATOM   1064  CD1 LEU A 236      33.979  57.968  -6.197  1.00  0.00           C
ATOM   1065  CD2 LEU A 236      34.012  55.479  -6.132  1.00  0.00           C
ATOM   1066  H   LEU A 236      32.058  56.073  -3.315  1.00  0.00           H
ATOM   1067  HA  LEU A 236      34.493  54.885  -3.715  1.00  0.00           H
ATOM   1068  1HB LEU A 236      34.052  57.769  -3.529  1.00  0.00           H
ATOM   1069  2HB LEU A 236      35.440  56.902  -4.228  1.00  0.00           H
ATOM   1070  HG  LEU A 236      32.560  56.695  -5.169  1.00  0.00           H
ATOM   1071  1HD1 LEU A 236     33.460  57.907  -7.153  1.00  0.00           H
ATOM   1072  2HD1 LEU A 236     33.669  58.872  -5.672  1.00  0.00           H
ATOM   1073  3HD1 LEU A 236     35.055  58.000  -6.370  1.00  0.00           H
ATOM   1074  1HD2 LEU A 236     33.461  55.456  -7.072  1.00  0.00           H
ATOM   1075  2HD2 LEU A 236     35.082  55.485  -6.338  1.00  0.00           H
ATOM   1076  3HD2 LEU A 236     33.760  54.596  -5.544  1.00  0.00           H
ATOM   1077  N   PRO A 237      34.501  56.633  -0.771  1.00  0.00           N
ATOM   1078  CA  PRO A 237      35.275  56.797   0.442  1.00  0.00           C
ATOM   1079  C   PRO A 237      35.127  55.560   1.325  1.00  0.00           C
ATOM   1080  O   PRO A 237      36.117  55.091   1.872  1.00  0.00           O
ATOM   1081  CB  PRO A 237      34.760  58.064   1.126  1.00  0.00           C
ATOM   1082  CG  PRO A 237      33.337  58.183   0.588  1.00  0.00           C
ATOM   1083  CD  PRO A 237      33.495  57.676  -0.844  1.00  0.00           C
ATOM   1084  HA  PRO A 237      36.320  56.970   0.186  1.00  0.00           H
ATOM   1085  1HB PRO A 237      34.792  57.933   2.207  1.00  0.00           H
ATOM   1086  2HB PRO A 237      35.388  58.910   0.844  1.00  0.00           H
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ATOM 1087 1HG PRO A 237 32.668 57.566 1.188 1.00 0.00 H
ATOM 1088 2HG PRO A 237 33.014 59.223 0.639 1.00 0.00 H
ATOM 1089 1HD PRO A 237 33.838 58.465 -1.513 1.00 0.00 H
ATOM 1090 2HD PRO A 237 32.564 57.257 -1.225 1.00 0.00 H
ATOM 1091 N ILE A 238 33.928 54.989 1.451 1.00 0.00 N
ATOM 1092 CA ILE A 238 33.752 53.784 2.251 1.00 0.00 C
ATOM 1093 C ILE A 238 34.655 52.676 1.715 1.00 0.00 C
ATOM 1094 O ILE A 238 35.204 51.894 2.488 1.00 0.00 O
ATOM 1095 CB ILE A 238 32.271 53.368 2.282 1.00 0.00 C
ATOM 1096 CGI ILE A 238 31.533 54.338 3.220 1.00 0.00 C
ATOM 1097 CG2 ILE A 238 32.062 51.919 2.744 1.00 0.00 C
ATOM 1098 CD1 ILE A 238 30.014 54.203 3.132 1.00 0.00 C
ATOM 1099 H ILE A 238 33.126 55.391 0.987 1.00 0.00 H
ATOM 1100 HA ILE A 238 33.939 54.013 3.300 1.00 0.00 H
ATOM 1101 HB ILE A 238 31.866 53.390 1.271 1.00 0.00 H
ATOM 1102 1HG1 ILE A 238 31.825 54.140 4.252 1.00 0.00 H
ATOM 1103 2HG1 ILE A 238 31.792 55.364 2.961 1.00 0.00 H
ATOM 1104 1HG2 ILE A 238 30.997 51.687 2.744 1.00 0.00 H
ATOM 1105 2HG2 ILE A 238 32.581 51.243 2.064 1.00 0.00 H
ATOM 1106 3HG2 ILE A 238 32.461 51.797 3.751 1.00 0.00 H
ATOM 1107 1HD1 ILE A 238 29.545 54.911 3.815 1.00 0.00 H
ATOM 1108 2HD1 ILE A 238 29.689 54.413 2.113 1.00 0.00 H
ATOM 1109 3HD1 ILE A 238 29.722 53.189 3.404 1.00 0.00 H
ATOM 1110 N LEU A 239 34.794 52.590 0.396 1.00 0.00 N
ATOM 1111 CA LEU A 239 35.675 51.620 -0.215 1.00 0.00 C
ATOM 1112 C LEU A 239 37.129 51.986 0.091 1.00 0.00 C
ATOM 1113 O LEU A 239 37.915 51.095 0.403 1.00 0.00 O
ATOM 1114 CB LEU A 239 35.365 51.493 -1.710 1.00 0.00 C
ATOM 1115 CG LEU A 239 33.980 50.862 -1.953 1.00 0.00 C
ATOM 1116 CD1 LEU A 239 33.526 51.171 -3.380 1.00 0.00 C
ATOM 1117 CD2 LEU A 239 33.994 49.340 -1.762 1.00 0.00 C
ATOM 1118 H LEU A 239 34.278 53.214 -0.208 1.00 0.00 H
ATOM 1119 HA LEU A 239 35.388 50.617 0.103 1.00 0.00 H
ATOM 1120 1HB LEU A 239 35.377 52.482 -2.168 1.00 0.00 H
ATOM 1121 2HB LEU A 239 36.118 50.864 -2.185 1.00 0.00 H
ATOM 1122 HG LEU A 239 33.265 51.267 -1.237 1.00 0.00 H
ATOM 1123 1HD1 LEU A 239 32.547 50.726 -3.555 1.00 0.00 H
ATOM 1124 2HD1 LEU A 239 33.463 52.251 -3.515 1.00 0.00 H
ATOM 1125 3HD1 LEU A 239 34.245 50.758 -4.088 1.00 0.00 H
ATOM 1126 1HD2 LEU A 239 32.996 48.941 -1.944 1.00 0.00 H
ATOM 1127 2HD2 LEU A 239 34.698 48.891 -2.464 1.00 0.00 H
ATOM 1128 3HD2 LEU A 239 34.299 49.103 -0.742 1.00 0.00 H
ATOM 1129 N SER A 240 37.490 53.274 0.067 1.00 0.00 N
ATOM 1130 CA SER A 240 38.789 53.711 0.567 1.00 0.00 C
ATOM 1131 C SER A 240 39.004 53.187 1.992 1.00 0.00 C
ATOM 1132 O SER A 240 40.069 52.659 2.297 1.00 0.00 O
ATOM 1133 CB SER A 240 38.956 55.242 0.509 1.00 0.00 C
ATOM 1134 OG SER A 240 40.271 55.647 0.866 1.00 0.00 O
ATOM 1135 H SER A 240 36.858 53.969 -0.304 1.00 0.00 H
ATOM 1136 HA SER A 240 39.571 53.389 -0.121 1.00 0.00 H
ATOM 1137 1HB SER A 240 38.756 55.592 -0.504 1.00 0.00 H
ATOM 1138 2HB SER A 240 38.256 55.711 1.200 1.00 0.00 H
ATOM 1139 HG SER A 240 40.335 56.604 0.818 1.00 0.00 H
ATOM 1140 N GLN A 241 37.997 53.276 2.865 1.00 0.00 N
ATOM 1141 CA GLN A 241 38.109 52.795 4.240 1.00 0.00 C
ATOM 1142 C GLN A 241 38.088 51.262 4.322 1.00 0.00 C
ATOM 1143 O GLN A 241 38.033 50.698 5.415 1.00 0.00 O
ATOM 1144 CB GLN A 241 37.005 53.369 5.135 1.00 0.00 C
ATOM 1145 CG GLN A 241 36.801 54.888 5.108 1.00 0.00 C

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ATOM   1146  CD  GLN A 241      38.015  55.722   5.492  1.00  0.00           C
ATOM   1147  NE2 GLN A 241      37.778  56.760   6.278  1.00  0.00           N
ATOM   1148  OE1 GLN A 241      39.140  55.495   5.043  1.00  0.00           O
ATOM   1149  H   GLN A 241      37.119  53.688   2.583  1.00  0.00           H
ATOM   1150  HA  GLN A 241      39.016  53.194   4.693  1.00  0.00           H
ATOM   1151  1HB GLN A 241      36.044  52.941   4.848  1.00  0.00           H
ATOM   1152  2HB GLN A 241      37.215  53.122   6.176  1.00  0.00           H
ATOM   1153  1HG GLN A 241      36.522  55.200   4.102  1.00  0.00           H
ATOM   1154  2HG GLN A 241      36.010  55.162   5.806  1.00  0.00           H
ATOM   1155  1HE2 GLN A 241     38.539  57.356   6.571  1.00  0.00           H
ATOM   1156  2HE2 GLN A 241     36.836  56.956   6.585  1.00  0.00           H
ATOM   1157  N   ILE A 242      38.115  50.566   3.186  1.00  0.00           N
ATOM   1158  CA  ILE A 242      38.313  49.133   3.115  1.00  0.00           C
ATOM   1159  C   ILE A 242      39.590  48.864   2.302  1.00  0.00           C
ATOM   1160  O   ILE A 242      40.084  47.735   2.277  1.00  0.00           O
ATOM   1161  CB  ILE A 242      37.045  48.444   2.563  1.00  0.00           C
ATOM   1162  CG1 ILE A 242      35.831  48.732   3.470  1.00  0.00           C
ATOM   1163  CG2 ILE A 242      37.255  46.924   2.491  1.00  0.00           C
ATOM   1164  CD1 ILE A 242      34.483  48.423   2.808  1.00  0.00           C
ATOM   1165  H   ILE A 242      37.992  51.039   2.302  1.00  0.00           H
ATOM   1166  HA  ILE A 242      38.313  48.715   4.121  1.00  0.00           H
ATOM   1167  HB  ILE A 242      36.836  48.816   1.560  1.00  0.00           H
ATOM   1168  1HG1 ILE A 242     35.897  48.123   4.372  1.00  0.00           H
ATOM   1169  2HG1 ILE A 242     35.824  49.787   3.745  1.00  0.00           H
ATOM   1170  1HG2 ILE A 242     36.355  46.450   2.100  1.00  0.00           H
ATOM   1171  2HG2 ILE A 242     38.096  46.703   1.833  1.00  0.00           H
ATOM   1172  3HG2 ILE A 242     37.464  46.538   3.489  1.00  0.00           H
ATOM   1173  1HD1 ILE A 242     33.675  48.650   3.504  1.00  0.00           H
ATOM   1174  2HD1 ILE A 242     34.370  49.032   1.911  1.00  0.00           H
ATOM   1175  3HD1 ILE A 242     34.443  47.368   2.537  1.00  0.00           H
ATOM   1176  N   TYR A 243      40.187  49.898   1.713  1.00  0.00           N
ATOM   1177  CA  TYR A 243      41.500  49.888   1.076  1.00  0.00           C
ATOM   1178  C   TYR A 243      42.446  50.665   1.998  1.00  0.00           C
ATOM   1179  O   TYR A 243      43.404  51.297   1.567  1.00  0.00           O
ATOM   1180  CB  TYR A 243      41.405  50.476  -0.342  1.00  0.00           C
ATOM   1181  CG  TYR A 243      40.296  49.900  -1.215  1.00  0.00           C
ATOM   1182  CD1 TYR A 243      39.827  48.584  -1.027  1.00  0.00           C
ATOM   1183  CD2 TYR A 243      39.693  50.684  -2.218  1.00  0.00           C
ATOM   1184  CE1 TYR A 243      38.738  48.097  -1.762  1.00  0.00           C
ATOM   1185  CE2 TYR A 243      38.632  50.178  -2.991  1.00  0.00           C
ATOM   1186  CZ  TYR A 243      38.136  48.881  -2.757  1.00  0.00           C
ATOM   1187  OH  TYR A 243      37.095  48.364  -3.474  1.00  0.00           O
ATOM   1188  H   TYR A 243      39.725  50.795   1.679  1.00  0.00           H
ATOM   1189  HA  TYR A 243      41.809  48.859   0.895  1.00  0.00           H
ATOM   1190  1HB TYR A 243      41.222  51.549  -0.280  1.00  0.00           H
ATOM   1191  2HB TYR A 243      42.340  50.298  -0.874  1.00  0.00           H
ATOM   1192  HD1 TYR A 243      40.307  47.937  -0.309  1.00  0.00           H
ATOM   1193  HD2 TYR A 243      40.045  51.689  -2.402  1.00  0.00           H
ATOM   1194  HE1 TYR A 243      38.352  47.108  -1.566  1.00  0.00           H
ATOM   1195  HE2 TYR A 243      38.193  50.785  -3.769  1.00  0.00           H
ATOM   1196  HH  TYR A 243      36.792  49.014  -4.112  1.00  0.00           H
ATOM   1197  N   SER A 244      42.129  50.577   3.288  1.00  0.00           N
ATOM   1198  CA  SER A 244      42.651  51.258   4.453  1.00  0.00           C
ATOM   1199  C   SER A 244      41.782  50.695   5.594  1.00  0.00           C
ATOM   1200  O   SER A 244      41.188  49.622   5.406  1.00  0.00           O
ATOM   1201  CB  SER A 244      42.512  52.779   4.288  1.00  0.00           C
ATOM   1202  OG  SER A 244      43.178  53.491   5.313  1.00  0.00           O
ATOM   1203  H   SER A 244      41.402  49.942   3.587  1.00  0.00           H
ATOM   1204  HA  SER A 244      43.710  51.028   4.564  1.00  0.00           H
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ATOM 1205 1HB SER A 244 42.940 53.082 3.332 1.00 0.00 H
ATOM 1206 2HB SER A 244 41.457 53.053 4.316 1.00 0.00 H
ATOM 1207 HG SER A 244 43.067 54.434 5.173 1.00 0.00 H
ATOM 1208 N ASP A 245 41.685 51.427 6.712 1.00 0.00 N
ATOM 1209 CA ASP A 245 40.956 51.110 7.948 1.00 0.00 C
ATOM 1210 C ASP A 245 40.531 49.642 8.056 1.00 0.00 C
ATOM 1211 O ASP A 245 41.306 48.823 8.551 1.00 0.00 O
ATOM 1212 CB ASP A 245 39.779 52.075 8.184 1.00 0.00 C
ATOM 1213 CG ASP A 245 38.905 51.658 9.368 1.00 0.00 C
ATOM 1214 OD1 ASP A 245 37.675 51.858 9.265 1.00 0.00 O
ATOM 1215 OD2 ASP A 245 39.448 51.130 10.358 1.00 0.00 Ol-
ATOM 1216 H ASP A 245 42.152 52.320 6.773 1.00 0.00 H
ATOM 1217 HA ASP A 245 41.525 51.465 8.807 1.00 0.00 H
ATOM 1218 1HB ASP A 245 40.163 53.075 8.387 1.00 0.00 H
ATOM 1219 2HB ASP A 245 39.148 52.103 7.296 1.00 0.00 H
ATOM 1220 N GLY A 246 39.306 49.342 7.601 1.00 0.00 N
ATOM 1221 CA GLY A 246 38.538 48.134 7.842 1.00 0.00 C
ATOM 1222 C GLY A 246 39.412 46.949 8.261 1.00 0.00 C
ATOM 1223 O GLY A 246 39.985 46.301 7.384 1.00 0.00 O
ATOM 1224 H GLY A 246 38.809 49.998 7.016 1.00 0.00 H
ATOM 1225 1HA GLY A 246 37.817 48.313 8.639 1.00 0.00 H
ATOM 1226 2HA GLY A 246 38.010 47.851 6.931 1.00 0.00 H
ATOM 1227 N PRO A 247 39.529 46.638 9.561 1.00 0.00 N
ATOM 1228 CA PRO A 247 40.711 45.918 10.008 1.00 0.00 C
ATOM 1229 C PRO A 247 40.835 44.482 9.482 1.00 0.00 C
ATOM 1230 O PRO A 247 39.901 43.901 8.924 1.00 0.00 O
ATOM 1231 CB PRO A 247 40.660 45.971 11.533 1.00 0.00 C
ATOM 1232 CG PRO A 247 40.095 47.370 11.770 1.00 0.00 C
ATOM 1233 CD PRO A 247 39.100 47.546 10.622 1.00 0.00 C
ATOM 1234 HA PRO A 247 41.604 46.484 9.742 1.00 0.00 H
ATOM 1235 1HB PRO A 247 40.012 45.177 11.904 1.00 0.00 H
ATOM 1236 2HB PRO A 247 41.664 45.838 11.936 1.00 0.00 H
ATOM 1237 1HG PRO A 247 39.614 47.407 12.747 1.00 0.00 H
ATOM 1238 2HG PRO A 247 40.904 48.099 11.736 1.00 0.00 H
ATOM 1239 1HD PRO A 247 39.112 48.571 10.250 1.00 0.00 H
ATOM 1240 2HD PRO A 247 38.090 47.286 10.938 1.00 0.00 H
ATOM 1241 N GLY A 248 42.024 43.910 9.657 1.00 0.00 N
ATOM 1242 CA GLY A 248 42.370 42.615 9.107 1.00 0.00 C
ATOM 1243 C GLY A 248 41.581 41.494 9.784 1.00 0.00 C
ATOM 1244 O GLY A 248 41.257 41.580 10.969 1.00 0.00 O
ATOM 1245 H GLY A 248 42.737 44.382 10.194 1.00 0.00 H
ATOM 1246 1HA GLY A 248 42.145 42.601 8.041 1.00 0.00 H
ATOM 1247 2HA GLY A 248 43.433 42.428 9.257 1.00 0.00 H
ATOM 1248 N GLU A 249 41.296 40.431 9.027 1.00 0.00 N
ATOM 1249 CA GLU A 249 40.608 39.234 9.483 1.00 0.00 C
ATOM 1250 C GLU A 249 41.125 38.752 10.845 1.00 0.00 C
ATOM 1251 O GLU A 249 40.334 38.388 11.711 1.00 0.00 O
ATOM 1252 CB GLU A 249 40.771 38.144 8.418 1.00 0.00 C
ATOM 1253 CG GLU A 249 39.870 38.408 7.198 1.00 0.00 C
ATOM 1254 CD GLU A 249 38.482 37.828 7.409 1.00 0.00 C
ATOM 1255 OE1 GLU A 249 37.474 38.559 7.315 1.00 0.00 O
ATOM 1256 OE2 GLU A 249 38.397 36.612 7.677 1.00 0.00 Ol-
ATOM 1257 H GLU A 249 41.564 40.417 8.053 1.00 0.00 H
ATOM 1258 HA GLU A 249 39.536 39.427 9.530 1.00 0.00 H
ATOM 1259 1HB GLU A 249 41.807 38.117 8.081 1.00 0.00 H
ATOM 1260 2HB GLU A 249 40.501 37.177 8.843 1.00 0.00 H
ATOM 1261 1HG GLU A 249 39.779 39.482 7.039 1.00 0.00 H
ATOM 1262 2HG GLU A 249 40.310 37.946 6.314 1.00 0.00 H
ATOM 1263 N ALA A 250 42.442 38.749 11.053 1.00 0.00 N

ATOM 1264 CA ALA A 250 43.035 38.279 12.298 1.00 0.00 C
ATOM 1265 C ALA A 250 42.938 39.368 13.373 1.00 0.00 C
ATOM 1266 O ALA A 250 43.952 39.820 13.892 1.00 0.00 O
ATOM 1267 CB ALA A 250 44.485 37.858 12.040 1.00 0.00 C
ATOM 1268 H ALA A 250 43.068 39.081 10.334 1.00 0.00 H
ATOM 1269 HA ALA A 250 42.542 37.358 12.611 1.00 0.00 H
ATOM 1270 1HB ALA A 250 44.933 37.506 12.970 1.00 0.00 H
ATOM 1271 2HB ALA A 250 44.506 37.057 11.301 1.00 0.00 H
ATOM 1272 3HB ALA A 250 45.051 38.712 11.666 1.00 0.00 H
ATOM 1273 N LEU A 251 41.711 39.766 13.711 1.00 0.00 N
ATOM 1274 CA LEU A 251 41.340 40.820 14.647 1.00 0.00 C
ATOM 1275 C LEU A 251 39.860 41.093 14.394 1.00 0.00 C
ATOM 1276 O LEU A 251 39.013 40.932 15.273 1.00 0.00 O
ATOM 1277 CB LEU A 251 42.185 42.097 14.465 1.00 0.00 C
ATOM 1278 CG LEU A 251 41.646 43.323 15.224 1.00 0.00 C
ATOM 1279 CD1 LEU A 251 41.547 43.066 16.733 1.00 0.00 C
ATOM 1280 CD2 LEU A 251 42.580 44.513 14.980 1.00 0.00 C
ATOM 1281 H LEU A 251 40.904 39.319 13.299 1.00 0.00 H
ATOM 1282 HA LEU A 251 41.539 40.487 15.666 1.00 0.00 H
ATOM 1283 1HB LEU A 251 43.198 41.918 14.826 1.00 0.00 H
ATOM 1284 2HB LEU A 251 42.218 42.364 13.409 1.00 0.00 H
ATOM 1285 HG LEU A 251 40.657 43.579 14.845 1.00 0.00 H
ATOM 1286 1HD1 LEU A 251 41.162 43.957 17.229 1.00 0.00 H
ATOM 1287 2HD1 LEU A 251 40.873 42.229 16.916 1.00 0.00 H
ATOM 1288 3HD1 LEU A 251 42.535 42.829 17.128 1.00 0.00 H
ATOM 1289 1HD2 LEU A 251 42.205 45.386 15.514 1.00 0.00 H
ATOM 1290 2HD2 LEU A 251 43.581 44.270 15.339 1.00 0.00 H
ATOM 1291 3HD2 LEU A 251 42.621 44.731 13.912 1.00 0.00 H
ATOM 1292 N ARG A 252 39.536 41.486 13.163 1.00 0.00 N
ATOM 1293 CA ARG A 252 38.164 41.678 12.738 1.00 0.00 C
ATOM 1294 C ARG A 252 37.433 40.346 12.894 1.00 0.00 C
ATOM 1295 O ARG A 252 36.567 40.203 13.760 1.00 0.00 O
ATOM 1296 CB ARG A 252 38.130 42.231 11.300 1.00 0.00 C
ATOM 1297 CG ARG A 252 36.728 42.437 10.704 1.00 0.00 C
ATOM 1298 CD ARG A 252 35.806 43.223 11.648 1.00 0.00 C
ATOM 1299 NE ARG A 252 34.663 43.874 10.982 1.00 0.00 N
ATOM 1300 CZ ARG A 252 33.713 43.337 10.203 1.00 0.00 C
ATOM 1301 NH1 ARG A 252 33.751 42.082 9.779 1.00 0.00 N1+
ATOM 1302 NH2 ARG A 252 32.695 44.110 9.855 1.00 0.00 N
ATOM 1303 H ARG A 252 40.260 41.663 12.482 1.00 0.00 H
ATOM 1304 HA ARG A 252 37.717 42.493 13.308 1.00 0.00 H
ATOM 1305 1HB ARG A 252 38.621 43.204 11.273 1.00 0.00 H
ATOM 1306 2HB ARG A 252 38.650 41.544 10.633 1.00 0.00 H
ATOM 1307 1HG ARG A 252 36.808 42.992 9.769 1.00 0.00 H
ATOM 1308 2HG ARG A 252 36.268 41.467 10.511 1.00 0.00 H
ATOM 1309 1HD ARG A 252 35.394 42.549 12.399 1.00 0.00 H
ATOM 1310 2HD ARG A 252 36.376 44.010 12.141 1.00 0.00 H
ATOM 1311 HE ARG A 252 34.652 44.864 11.183 1.00 0.00 H
ATOM 1312 1HH1 ARG A 252 33.010 41.724 9.193 1.00 0.00 H
ATOM 1313 2HH1 ARG A 252 34.520 41.483 10.043 1.00 0.00 H
ATOM 1314 1HH2 ARG A 252 31.960 43.742 9.268 1.00 0.00 H
ATOM 1315 2HH2 ARG A 252 32.655 45.066 10.175 1.00 0.00 H
ATOM 1316 N ALA A 253 37.834 39.370 12.086 1.00 0.00 N
ATOM 1317 CA ALA A 253 37.093 38.115 11.840 1.00 0.00 C
ATOM 1318 C ALA A 253 37.464 37.033 12.804 1.00 0.00 C
ATOM 1319 O ALA A 253 36.935 35.926 12.718 1.00 0.00 O
ATOM 1320 CB ALA A 253 37.275 37.724 10.394 1.00 0.00 C
ATOM 1321 H ALA A 253 38.712 39.452 11.593 1.00 0.00 H
ATOM 1322 HA ALA A 253 36.024 38.363 11.863 1.00 0.00 H

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ATOM   1323 1HB  ALA A 253     36.716  36.806  10.213  1.00  0.00          H
ATOM   1324 2HB  ALA A 253     36.907  38.509   9.734  1.00  0.00          H
ATOM   1325 3HB  ALA A 253     38.333  37.549  10.197  1.00  0.00          H
ATOM   1326  N   MET A 254     38.308  37.342  13.785  1.00  0.00          N
ATOM   1327  CA  MET A 254     38.657  36.439  14.874  1.00  0.00          C
ATOM   1328  C   MET A 254     37.545  36.461  15.934  1.00  0.00          C
ATOM   1329  O   MET A 254     37.755  36.101  17.086  1.00  0.00          O
ATOM   1330  CB  MET A 254     40.036  36.850  15.416  1.00  0.00          C
ATOM   1331  CG  MET A 254     40.671  35.803  16.341  1.00  0.00          C
ATOM   1332  SD  MET A 254     42.466  35.962  16.549  1.00  0.00          S
ATOM   1333  CE  MET A 254     42.576  37.617  17.275  1.00  0.00          C
ATOM   1334  H   MET A 254     38.750  38.249  13.805  1.00  0.00          H
ATOM   1335  HA  MET A 254     38.846  35.443  14.474  1.00  0.00          H
ATOM   1336 1HB  MET A 254     40.723  37.006  14.584  1.00  0.00          H
ATOM   1337 2HB  MET A 254     39.942  37.773  15.988  1.00  0.00          H
ATOM   1338 1HG  MET A 254     40.231  35.882  17.336  1.00  0.00          H
ATOM   1339 2HG  MET A 254     40.487  34.805  15.942  1.00  0.00          H
ATOM   1340 1HE  MET A 254     43.621  37.864  17.463  1.00  0.00          H
ATOM   1341 2HE  MET A 254     42.149  38.346  16.586  1.00  0.00          H
ATOM   1342 3HE  MET A 254     42.024  37.640  18.215  1.00  0.00          H
ATOM   1343  N   LYS A 255     36.355  36.928  15.553  1.00  0.00          N
ATOM   1344  CA  LYS A 255     35.141  36.968  16.344  1.00  0.00          C
ATOM   1345  C   LYS A 255     33.964  36.658  15.404  1.00  0.00          C
ATOM   1346  O   LYS A 255     32.823  37.036  15.679  1.00  0.00          O
ATOM   1347  CB  LYS A 255     34.994  38.381  16.929  1.00  0.00          C
ATOM   1348  CG  LYS A 255     36.217  38.839  17.745  1.00  0.00          C
ATOM   1349  CD  LYS A 255     36.040  40.245  18.342  1.00  0.00          C
ATOM   1350  CE  LYS A 255     36.542  41.380  17.431  1.00  0.00          C
ATOM   1351  NZ  LYS A 255     35.939  41.383  16.080  1.00  0.00          N1+
ATOM   1352  H   LYS A 255     36.234  37.305  14.624  1.00  0.00          H
ATOM   1353  HA  LYS A 255     35.192  36.212  17.128  1.00  0.00          H
ATOM   1354 1HB  LYS A 255     34.856  39.098  16.120  1.00  0.00          H
ATOM   1355 2HB  LYS A 255     34.130  38.412  17.593  1.00  0.00          H
ATOM   1356 1HG  LYS A 255     36.384  38.146  18.570  1.00  0.00          H
ATOM   1357 2HG  LYS A 255     37.097  38.858  17.102  1.00  0.00          H
ATOM   1358 1HD  LYS A 255     34.982  40.429  18.532  1.00  0.00          H
ATOM   1359 2HD  LYS A 255     36.594  40.316  19.278  1.00  0.00          H
ATOM   1360 1HE  LYS A 255     36.309  42.343  17.887  1.00  0.00          H
ATOM   1361 2HE  LYS A 255     37.620  41.292  17.299  1.00  0.00          H
ATOM   1362 1HZ  LYS A 255     36.315  42.152  15.545  1.00  0.00          H
ATOM   1363 2HZ  LYS A 255     36.152  40.513  15.614  1.00  0.00          H
ATOM   1364 3HZ  LYS A 255     34.937  41.487  16.159  1.00  0.00          H
ATOM   1365  N   GLU A 256     34.261  36.044  14.253  1.00  0.00          N
ATOM   1366  CA  GLU A 256     33.325  35.873  13.152  1.00  0.00          C
ATOM   1367  C   GLU A 256     33.543  34.516  12.478  1.00  0.00          C
ATOM   1368  O   GLU A 256     32.590  33.821  12.128  1.00  0.00          O
ATOM   1369  CB  GLU A 256     33.535  36.973  12.101  1.00  0.00          C
ATOM   1370  CG  GLU A 256     33.583  38.410  12.642  1.00  0.00          C
ATOM   1371  CD  GLU A 256     33.830  39.416  11.529  1.00  0.00          C
ATOM   1372  OE1 GLU A 256     33.712  39.055  10.338  1.00  0.00          O
ATOM   1373  OE2 GLU A 256     34.210  40.555  11.859  1.00  0.00          O1-
ATOM   1374  H   GLU A 256     35.186  35.663  14.108  1.00  0.00          H
ATOM   1375  HA  GLU A 256     32.304  35.913  13.533  1.00  0.00          H
ATOM   1376 1HB  GLU A 256     34.482  36.808  11.587  1.00  0.00          H
ATOM   1377 2HB  GLU A 256     32.721  36.945  11.377  1.00  0.00          H
ATOM   1378 1HG  GLU A 256     32.633  38.651  13.120  1.00  0.00          H
ATOM   1379 2HG  GLU A 256     34.389  38.498  13.371  1.00  0.00          H
ATOM   1380  N   ASN A 257     34.807  34.167  12.242  1.00  0.00          N
ATOM   1381  CA  ASN A 257     35.170  32.955  11.524  1.00  0.00          C
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ATOM   1382  C   ASN A 257      35.106  31.772  12.482  1.00  0.00           C
ATOM   1383  O   ASN A 257      35.577  31.866  13.614  1.00  0.00           O
ATOM   1384  CB  ASN A 257      36.591  33.059  10.949  1.00  0.00           C
ATOM   1385  CG  ASN A 257      36.670  33.920   9.693  1.00  0.00           C
ATOM   1386  ND2 ASN A 257      37.779  34.628   9.505  1.00  0.00           N
ATOM   1387  OD1 ASN A 257      35.740  33.948   8.886  1.00  0.00           O
ATOM   1388  H   ASN A 257      35.562  34.754  12.566  1.00  0.00           H
ATOM   1389  HA  ASN A 257      34.475  32.800  10.698  1.00  0.00           H
ATOM   1390 1HB  ASN A 257      37.253  33.502  11.694  1.00  0.00           H
ATOM   1391 2HB  ASN A 257      36.952  32.064  10.689  1.00  0.00           H
ATOM   1392 1HD2 ASN A 257      37.872  35.211  8.686  1.00  0.00           H
ATOM   1393 2HD2 ASN A 257      38.528  34.583  10.181  1.00  0.00           H
ATOM   1394  N   GLY A 258      34.585  30.635  12.029  1.00  0.00           N
ATOM   1395  CA  GLY A 258      34.511  29.443  12.846  1.00  0.00           C
ATOM   1396  C   GLY A 258      34.104  28.232  12.007  1.00  0.00           C
ATOM   1397  O   GLY A 258      34.342  28.189  10.802  1.00  0.00           O
ATOM   1398  H   GLY A 258      34.225  30.585  11.086  1.00  0.00           H
ATOM   1399 1HA  GLY A 258      35.485  29.248  13.294  1.00  0.00           H
ATOM   1400 2HA  GLY A 258      33.772  29.588  13.634  1.00  0.00           H
ATOM   1401  N   ARG A 259      33.484  27.236  12.648  1.00  0.00           N
ATOM   1402  CA  ARG A 259      33.355  25.871  12.142  1.00  0.00           C
ATOM   1403  C   ARG A 259      32.606  25.760  10.805  1.00  0.00           C
ATOM   1404  O   ARG A 259      32.595  24.688  10.208  1.00  0.00           O
ATOM   1405  CB  ARG A 259      32.692  25.013  13.241  1.00  0.00           C
ATOM   1406  CG  ARG A 259      32.557  23.520  12.895  1.00  0.00           C
ATOM   1407  CD  ARG A 259      32.041  22.693  14.083  1.00  0.00           C
ATOM   1408  NE  ARG A 259      33.046  22.541  15.154  1.00  0.00           N
ATOM   1409  CZ  ARG A 259      34.012  21.609  15.189  1.00  0.00           C
ATOM   1410  NH1 ARG A 259      34.204  20.817  14.131  1.00  0.00           N1+
ATOM   1411  NH2 ARG A 259      34.775  21.484  16.276  1.00  0.00           N
ATOM   1412  H   ARG A 259      33.063  27.401  13.551  1.00  0.00           H
ATOM   1413  HA  ARG A 259      34.342  25.412  12.074  1.00  0.00           H
ATOM   1414 1HB  ARG A 259      33.283  25.073  14.155  1.00  0.00           H
ATOM   1415 2HB  ARG A 259      31.686  25.384  13.435  1.00  0.00           H
ATOM   1416 1HG  ARG A 259      31.855  23.400  12.070  1.00  0.00           H
ATOM   1417 2HG  ARG A 259      33.530  23.124  12.604  1.00  0.00           H
ATOM   1418 1HD  ARG A 259      31.168  23.181  14.514  1.00  0.00           H
ATOM   1419 2HD  ARG A 259      31.767  21.695  13.740  1.00  0.00           H
ATOM   1420  HE  ARG A 259      32.966  23.213  15.903  1.00  0.00           H
ATOM   1421 1HH1 ARG A 259      34.929  20.114  14.152  1.00  0.00           H
ATOM   1422 2HH1 ARG A 259      33.624  20.921  13.311  1.00  0.00           H
ATOM   1423 1HH2 ARG A 259      35.502  20.784  16.306  1.00  0.00           H
ATOM   1424 2HH2 ARG A 259      34.624  22.090  17.071  1.00  0.00           H
ATOM   1425  N   TYR A 260      31.950  26.824  10.344  1.00  0.00           N
ATOM   1426  CA  TYR A 260      31.140  26.805   9.134  1.00  0.00           C
ATOM   1427  C   TYR A 260      31.498  28.025   8.282  1.00  0.00           C
ATOM   1428  O   TYR A 260      30.663  28.577   7.560  1.00  0.00           O
ATOM   1429  CB  TYR A 260      29.655  26.799   9.526  1.00  0.00           C
ATOM   1430  CG  TYR A 260      29.302  25.790  10.604  1.00  0.00           C
ATOM   1431  CD1 TYR A 260      29.391  24.410  10.348  1.00  0.00           C
ATOM   1432  CD2 TYR A 260      28.906  26.215  11.888  1.00  0.00           C
ATOM   1433  CE1 TYR A 260      29.113  23.473  11.358  1.00  0.00           C
ATOM   1434  CE2 TYR A 260      28.618  25.279  12.896  1.00  0.00           C
ATOM   1435  CZ  TYR A 260      28.732  23.900  12.643  1.00  0.00           C
ATOM   1436  OH  TYR A 260      28.473  22.980  13.619  1.00  0.00           O
ATOM   1437  H   TYR A 260      32.000  27.701  10.841  1.00  0.00           H
ATOM   1438  HA  TYR A 260      31.312  25.874   8.595  1.00  0.00           H
ATOM   1439 1HB  TYR A 260      29.374  27.782   9.903  1.00  0.00           H
ATOM   1440 2HB  TYR A 260      29.049  26.558   8.652  1.00  0.00           H
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ATOM   1441  HD1 TYR A 260      29.675  24.060   9.366  1.00  0.00           H
ATOM   1442  HD2 TYR A 260      28.820  27.269  12.105  1.00  0.00           H
ATOM   1443  HE1 TYR A 260      29.190  22.416  11.151  1.00  0.00           H
ATOM   1444  HE2 TYR A 260      28.306  25.617  13.873  1.00  0.00           H
ATOM   1445  HH  TYR A 260      28.228  23.434  14.429  1.00  0.00           H
ATOM   1446  N   GLY A 261      32.734  28.501   8.417  1.00  0.00           N
ATOM   1447  CA  GLY A 261      33.154  29.737   7.794  1.00  0.00           C
ATOM   1448  C   GLY A 261      32.597  30.873   8.642  1.00  0.00           C
ATOM   1449  O   GLY A 261      33.032  31.050   9.774  1.00  0.00           O
ATOM   1450  H   GLY A 261      33.412  27.996   8.968  1.00  0.00           H
ATOM   1451  1HA GLY A 261      34.243  29.777   7.763  1.00  0.00           H
ATOM   1452  2HA GLY A 261      32.761  29.785   6.778  1.00  0.00           H
ATOM   1453  N   ARG A 262      31.614  31.607   8.124  1.00  0.00           N
ATOM   1454  CA  ARG A 262      31.027  32.770   8.770  1.00  0.00           C
ATOM   1455  C   ARG A 262      29.536  32.685   8.444  1.00  0.00           C
ATOM   1456  O   ARG A 262      29.192  32.612   7.265  1.00  0.00           O
ATOM   1457  CB  ARG A 262      31.701  34.022   8.176  1.00  0.00           C
ATOM   1458  CG  ARG A 262      31.519  35.299   9.014  1.00  0.00           C
ATOM   1459  CD  ARG A 262      32.409  36.460   8.526  1.00  0.00           C
ATOM   1460  NE  ARG A 262      33.830  36.074   8.473  1.00  0.00           N
ATOM   1461  CZ  ARG A 262      34.835  36.815   7.989  1.00  0.00           C
ATOM   1462  NH1 ARG A 262      34.864  38.138   8.095  1.00  0.00           N1+
ATOM   1463  NH2 ARG A 262      35.825  36.172   7.393  1.00  0.00           N
ATOM   1464  H   ARG A 262      31.226  31.367   7.223  1.00  0.00           H
ATOM   1465  HA  ARG A 262      31.216  32.725   9.843  1.00  0.00           H
ATOM   1466  1HB ARG A 262      32.774  33.850   8.087  1.00  0.00           H
ATOM   1467  2HB ARG A 262      31.284  34.227   7.190  1.00  0.00           H
ATOM   1468  1HG ARG A 262      30.481  35.627   8.958  1.00  0.00           H
ATOM   1469  2HG ARG A 262      31.779  35.093  10.053  1.00  0.00           H
ATOM   1470  1HD ARG A 262      32.099  36.760   7.525  1.00  0.00           H
ATOM   1471  2HD ARG A 262      32.309  37.306   9.205  1.00  0.00           H
ATOM   1472  HE  ARG A 262      34.015  35.155   8.849  1.00  0.00           H
ATOM   1473  1HH1 ARG A 262      35.642  38.659   7.716  1.00  0.00           H
ATOM   1474  2HH1 ARG A 262      34.108  38.624   8.556  1.00  0.00           H
ATOM   1475  1HH2 ARG A 262      36.605  36.688   7.012  1.00  0.00           H
ATOM   1476  2HH2 ARG A 262      35.800  35.165   7.319  1.00  0.00           H
ATOM   1477  N   ARG A 263      28.668  32.603   9.456  1.00  0.00           N
ATOM   1478  CA  ARG A 263      27.229  32.403   9.282  1.00  0.00           C
ATOM   1479  C   ARG A 263      26.514  33.727   9.531  1.00  0.00           C
ATOM   1480  O   ARG A 263      25.837  34.245   8.644  1.00  0.00           O
ATOM   1481  CB  ARG A 263      26.698  31.325  10.238  1.00  0.00           C
ATOM   1482  CG  ARG A 263      27.330  29.936  10.075  1.00  0.00           C
ATOM   1483  CD  ARG A 263      27.035  29.280   8.717  1.00  0.00           C
ATOM   1484  NE  ARG A 263      28.105  29.532   7.736  1.00  0.00           N
ATOM   1485  CZ  ARG A 263      27.998  30.051   6.504  1.00  0.00           C
ATOM   1486  NH1 ARG A 263      26.877  30.604   6.064  1.00  0.00           N1+
ATOM   1487  NH2 ARG A 263      29.058  29.990   5.701  1.00  0.00           N
ATOM   1488  H   ARG A 263      28.994  32.678  10.409  1.00  0.00           H
ATOM   1489  HA  ARG A 263      27.033  32.033   8.276  1.00  0.00           H
ATOM   1490  1HB ARG A 263      26.881  31.630  11.268  1.00  0.00           H
ATOM   1491  2HB ARG A 263      25.627  31.198  10.082  1.00  0.00           H
ATOM   1492  1HG ARG A 263      28.413  30.016  10.168  1.00  0.00           H
ATOM   1493  2HG ARG A 263      26.948  29.269  10.848  1.00  0.00           H
ATOM   1494  1HD ARG A 263      26.940  28.202   8.846  1.00  0.00           H
ATOM   1495  2HD ARG A 263      26.105  29.681   8.314  1.00  0.00           H
ATOM   1496  HE  ARG A 263      29.010  29.259   8.092  1.00  0.00           H
ATOM   1497  1HH1 ARG A 263      26.835  30.985   5.130  1.00  0.00           H
ATOM   1498  2HH1 ARG A 263      26.065  30.646   6.664  1.00  0.00           H
ATOM   1499  1HH2 ARG A 263      29.007  30.372   4.768  1.00  0.00           H
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ATOM   1500 2HH2 ARG A 263      29.913  29.561   6.026  1.00  0.00           H
ATOM   1501  N   LYS A 264      26.700  34.292  10.726  1.00  0.00           N
ATOM   1502  CA  LYS A 264      26.332  35.676  10.943  1.00  0.00           C
ATOM   1503  C   LYS A 264      27.344  36.469  10.123  1.00  0.00           C
ATOM   1504  O   LYS A 264      28.542  36.342  10.367  1.00  0.00           O
ATOM   1505  CB  LYS A 264      26.378  36.024  12.447  1.00  0.00           C
ATOM   1506  CG  LYS A 264      25.692  37.374  12.710  1.00  0.00           C
ATOM   1507  CD  LYS A 264      25.573  37.788  14.191  1.00  0.00           C
ATOM   1508  CE  LYS A 264      26.905  38.243  14.813  1.00  0.00           C
ATOM   1509  NZ  LYS A 264      26.721  39.257  15.877  1.00  0.00           N1+
ATOM   1510  H   LYS A 264      27.099  33.754  11.482  1.00  0.00           H
ATOM   1511  HA  LYS A 264      25.301  35.833  10.623  1.00  0.00           H
ATOM   1512 1HB  LYS A 264      25.863  35.250  13.015  1.00  0.00           H
ATOM   1513 2HB  LYS A 264      27.416  36.085  12.774  1.00  0.00           H
ATOM   1514 1HG  LYS A 264      26.252  38.168  12.216  1.00  0.00           H
ATOM   1515 2HG  LYS A 264      24.676  37.348  12.318  1.00  0.00           H
ATOM   1516 1HD  LYS A 264      24.872  38.618  14.281  1.00  0.00           H
ATOM   1517 2HD  LYS A 264      25.212  36.943  14.777  1.00  0.00           H
ATOM   1518 1HE  LYS A 264      27.412  37.385  15.254  1.00  0.00           H
ATOM   1519 2HE  LYS A 264      27.537  38.681  14.041  1.00  0.00           H
ATOM   1520 1HZ  LYS A 264      27.622  39.520  16.251  1.00  0.00           H
ATOM   1521 2HZ  LYS A 264      26.266  40.072  15.492  1.00  0.00           H
ATOM   1522 3HZ  LYS A 264      26.151  38.871  16.616  1.00  0.00           H
ATOM   1523  N   GLN A 265      26.891  37.231  9.132  1.00  0.00           N
ATOM   1524  CA  GLN A 265      27.785  38.053  8.341  1.00  0.00           C
ATOM   1525  C   GLN A 265      27.992  39.361  9.097  1.00  0.00           C
ATOM   1526  O   GLN A 265      27.061  39.849  9.738  1.00  0.00           O
ATOM   1527  CB  GLN A 265      27.194  38.313  6.951  1.00  0.00           C
ATOM   1528  CG  GLN A 265      26.746  37.025  6.249  1.00  0.00           C
ATOM   1529  CD  GLN A 265      27.871  36.005  6.162  1.00  0.00           C
ATOM   1530  NE2 GLN A 265      27.617  34.781  6.600  1.00  0.00           N
ATOM   1531  OE1 GLN A 265      28.981  36.327  5.747  1.00  0.00           O
ATOM   1532  H   GLN A 265      25.905  37.246  8.917  1.00  0.00           H
ATOM   1533  HA  GLN A 265      28.727  37.526  8.192  1.00  0.00           H
ATOM   1534 1HB  GLN A 265      26.325  38.964  7.042  1.00  0.00           H
ATOM   1535 2HB  GLN A 265      27.943  38.793  6.322  1.00  0.00           H
ATOM   1536 1HG  GLN A 265      25.921  36.577  6.803  1.00  0.00           H
ATOM   1537 2HG  GLN A 265      26.418  37.258  5.236  1.00  0.00           H
ATOM   1538 1HE2 GLN A 265      28.334  34.071  6.562  1.00  0.00           H
ATOM   1539 2HE2 GLN A 265      26.705  34.557  6.973  1.00  0.00           H
ATOM   1540  N   TYR A 266      29.190  39.932  8.998  1.00  0.00           N
ATOM   1541  CA  TYR A 266      29.557  41.156  9.686  1.00  0.00           C
ATOM   1542  C   TYR A 266      30.053  42.140  8.623  1.00  0.00           C
ATOM   1543  O   TYR A 266      31.265  42.250  8.411  1.00  0.00           O
ATOM   1544  CB  TYR A 266      30.673  40.871  10.700  1.00  0.00           C
ATOM   1545  CG  TYR A 266      30.363  39.910  11.831  1.00  0.00           C
ATOM   1546  CD1 TYR A 266      30.196  40.375  13.149  1.00  0.00           C
ATOM   1547  CD2 TYR A 266      30.313  38.524  11.597  1.00  0.00           C
ATOM   1548  CE1 TYR A 266      30.089  39.469  14.217  1.00  0.00           C
ATOM   1549  CE2 TYR A 266      30.173  37.618  12.660  1.00  0.00           C
ATOM   1550  CZ  TYR A 266      30.113  38.082  13.984  1.00  0.00           C
ATOM   1551  OH  TYR A 266      30.116  37.198  15.024  1.00  0.00           O
ATOM   1552  H   TYR A 266      29.904  39.512  8.420  1.00  0.00           H
ATOM   1553  HA  TYR A 266      28.685  41.562  10.198  1.00  0.00           H
ATOM   1554 1HB  TYR A 266      31.531  40.440  10.184  1.00  0.00           H
ATOM   1555 2HB  TYR A 266      30.970  41.800  11.185  1.00  0.00           H
ATOM   1556  HD1 TYR A 266      30.150  41.436  13.345  1.00  0.00           H
ATOM   1557  HD2 TYR A 266      30.383  38.145  10.588  1.00  0.00           H
ATOM   1558  HE1 TYR A 266      29.988  39.835  15.228  1.00  0.00           H
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ATOM   1559  HE2 TYR A 266      30.111  36.558  12.461  1.00  0.00           H
ATOM   1560  HH  TYR A 266      30.133  36.301  14.682  1.00  0.00           H
ATOM   1561  N   PRO A 267      29.152  42.855   7.935  1.00  0.00           N
ATOM   1562  CA  PRO A 267      29.511  43.887   6.976  1.00  0.00           C
ATOM   1563  C   PRO A 267      30.521  44.868   7.579  1.00  0.00           C
ATOM   1564  O   PRO A 267      30.426  45.206   8.758  1.00  0.00           O
ATOM   1565  CB  PRO A 267      28.198  44.599   6.623  1.00  0.00           C
ATOM   1566  CG  PRO A 267      27.115  43.585   6.983  1.00  0.00           C
ATOM   1567  CD  PRO A 267      27.723  42.882   8.192  1.00  0.00           C
ATOM   1568  HA  PRO A 267      29.949  43.426   6.091  1.00  0.00           H
ATOM   1569 1HB  PRO A 267      28.112  45.514   7.208  1.00  0.00           H
ATOM   1570 2HB  PRO A 267      28.192  44.845   5.561  1.00  0.00           H
ATOM   1571  IHG  PRO A 267      26.189  44.110   7.217  1.00  0.00           H
ATOM   1572 2HG  PRO A 267      26.949  42.915   6.139  1.00  0.00           H
ATOM   1573  IHD  PRO A 267      27.352  41.862   8.291  1.00  0.00           H
ATOM   1574 2HD  PRO A 267      27.529  43.430   9.114  1.00  0.00           H
ATOM   1575  N   ILE A 268      31.512  45.308   6.807  1.00  0.00           N
ATOM   1576  CA  ILE A 268      32.443  46.334   7.260  1.00  0.00           C
ATOM   1577  C   ILE A 268      31.731  47.690   7.203  1.00  0.00           C
ATOM   1578  O   ILE A 268      32.121  48.629   7.895  1.00  0.00           O
ATOM   1579  CB  ILE A 268      33.746  46.290   6.430  1.00  0.00           C
ATOM   1580  CGI ILE A 268      34.351  44.870   6.451  1.00  0.00           C
ATOM   1581  CG2 ILE A 268      34.759  47.303   6.989  1.00  0.00           C
ATOM   1582  CD1 ILE A 268      35.575  44.712   5.541  1.00  0.00           C
ATOM   1583  H   ILE A 268      31.635  44.930   5.878  1.00  0.00           H
ATOM   1584  HA  ILE A 268      32.820  46.073   8.248  1.00  0.00           H
ATOM   1585  HB  ILE A 268      33.535  46.596   5.405  1.00  0.00           H
ATOM   1586 1HG1 ILE A 268      34.666  44.623   7.466  1.00  0.00           H
ATOM   1587 2HG1 ILE A 268      33.603  44.150   6.119  1.00  0.00           H
ATOM   1588 1HG2 ILE A 268      35.675  47.265   6.399  1.00  0.00           H
ATOM   1589 2HG2 ILE A 268      34.337  48.306   6.939  1.00  0.00           H
ATOM   1590 3HG2 ILE A 268      34.986  47.056   8.026  1.00  0.00           H
ATOM   1591 1HD1 ILE A 268      35.948  43.690   5.606  1.00  0.00           H
ATOM   1592 2HD1 ILE A 268      35.293  44.931   4.511  1.00  0.00           H
ATOM   1593 3HD1 ILE A 268      36.355  45.404   5.858  1.00  0.00           H
ATOM   1594  N   SER A 269      30.681  47.766   6.387  1.00  0.00           N
ATOM   1595  CA  SER A 269      29.879  48.948   6.168  1.00  0.00           C
ATOM   1596  C   SER A 269      28.470  48.482   5.804  1.00  0.00           C
ATOM   1597  O   SER A 269      28.315  47.433   5.170  1.00  0.00           O
ATOM   1598  CB  SER A 269      30.498  49.773   5.035  1.00  0.00           C
ATOM   1599  OG  SER A 269      29.790  50.985   4.880  1.00  0.00           O
ATOM   1600  H   SER A 269      30.390  46.954   5.861  1.00  0.00           H
ATOM   1601  HA  SER A 269      29.869  49.554   7.074  1.00  0.00           H
ATOM   1602 1HB  SER A 269      31.539  49.993   5.273  1.00  0.00           H
ATOM   1603 2HB  SER A 269      30.450  49.207   4.105  1.00  0.00           H
ATOM   1604  HG  SER A 269      30.183  51.497   4.169  1.00  0.00           H
ATOM   1605  N   LEU A 270      27.464  49.251   6.209  1.00  0.00           N
ATOM   1606  CA  LEU A 270      26.055  48.970   6.010  1.00  0.00           C
ATOM   1607  C   LEU A 270      25.412  50.219   5.421  1.00  0.00           C
ATOM   1608  O   LEU A 270      25.711  51.328   5.861  1.00  0.00           O
ATOM   1609  CB  LEU A 270      25.418  48.644   7.369  1.00  0.00           C
ATOM   1610  CG  LEU A 270      23.879  48.580   7.341  1.00  0.00           C
ATOM   1611 CD1 LEU A 270      23.363  47.417   6.484  1.00  0.00           C
ATOM   1612 CD2 LEU A 270      23.364  48.418   8.770  1.00  0.00           C
ATOM   1613  H   LEU A 270      27.653  50.113   6.701  1.00  0.00           H
ATOM   1614  HA  LEU A 270      25.945  48.138   5.313  1.00  0.00           H
ATOM   1615 1HB  LEU A 270      25.774  47.673   7.714  1.00  0.00           H
ATOM   1616 2HB  LEU A 270      25.694  49.410   8.093  1.00  0.00           H
ATOM   1617  HG  LEU A 270      23.483  49.514   6.942  1.00  0.00           H
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ATOM   1618 1HD1 LEU A 270     22.273  47.413   6.494  1.00  0.00           H
ATOM   1619 2HD1 LEU A 270     23.716  47.535   5.459  1.00  0.00           H
ATOM   1620 3HD1 LEU A 270     23.734  46.475   6.888  1.00  0.00           H
ATOM   1621  1HD2 LEU A 270     22.275  48.372   8.761  1.00  0.00           H
ATOM   1622 2HD2 LEU A 270     23.763  47.499   9.199  1.00  0.00           H
ATOM   1623 3HD2 LEU A 270     23.686  49.268   9.371  1.00  0.00           H
ATOM   1624  N   VAL A 271     24.498  50.036   4.473  1.00  0.00           N
ATOM   1625  CA  VAL A 271     23.71 1  5 1.1 17   3.914  1.00  0.00           C
ATOM   1626  C   VAL A 271     22.229  50.773   4.083  1.00  0.00           C
ATOM   1627  O   VAL A 271     21.823  49.632   3.853  1.00  0.00           O
ATOM   1628  CB  VAL A 271     24.085  5 1.329   2.439  1.00  0.00           C
ATOM   1629  CGI VAL A 271     23.370  52.577   1.902  1.00  0.00           C
ATOM   1630  CG2 VAL A 271     25.606  5 1.430   2.229  1.00  0.00           C
ATOM   163 1 H   VAL A 271     24.325  49. 110   4.109  1.00  0.00           H
ATOM   1632  HA  VAL A 271     23.974  52.052   4.408  1.00  0.00           H
ATOM   1633  HB  VAL A 271     23.847  50.43 1   1.870  1.00  0.00           H
ATOM   1634 1HG1 VAL A 271     23.636  52.728   0.856  1.00  0.00           H
ATOM   1635 2HG1 VAL A 271     22.291  52.443   1.986  1.00  0.00           H
ATOM   1636 3HG1 VAL A 271     23.673  53.449   2.482  1.00  0.00           H
ATOM   1637  1HG2 VAL A 271     25.818  5 1.580   1.171  1.00  0.00           H
ATOM   1638 2HG2 VAL A 271     25.997  52.272   2.801  1.00  0.00           H
ATOM   1639 3HG2 VAL A 271     26.081  50.509   2.568  1.00  0.00           H
ATOM   1640  N   LEU A 272     2 1.424  5 1.756   4.471  1.00  0.00           N
ATOM   1641  CA  LEU A 272     19.987  5 1.629   4.621  1.00  0.00           C
ATOM   1642  C   LEU A 272     19.3 16  52.516   3.576  1.00  0.00           C
ATOM   1643  O   LEU A 272     19.849  53.562   3.210  1.00  0.00           O
ATOM   1644  CB  LEU A 272     19.562  52.039   6.037  1.00  0.00           C
ATOM   1645  CG  LEU A 272     20. 189  5 1. 192   7. 156  1.00  0.00           C
ATOM   1646  CD1 LEU A 272     19.724  5 1.728   8.5 16  1.00  0.00           C
ATOM   1647  CD2 LEU A 272     19.798  49.714   7.037  1.00  0.00           C
ATOM   1648  H   LEU A 272     2 1.805  52.667   4.683  1.00  0.00           H
ATOM   1649  HA  LEU A 272     19.699  50.585   4.495  1.00  0.00           H
ATOM   1650  1HB  LEU A 272     19.854  53.073   6.219  1.00  0.00           H
ATOM   1651  2HB  LEU A 272     18.481  5 1.945   6.134  1.00  0.00           H
ATOM   1652  HG  LEU A 272     21.276  5 1.238   7.082  1.00  0.00           H
ATOM   1653 1HD1 LEU A 272     20.166  5 1.130   9.3 13  1.00  0.00           H
ATOM   1654 2HD1 LEU A 272     20.038  52.766   8.624  1.00  0.00           H
ATOM   1655 3HD1 LEU A 272     18.638  5 1.669   8.578  1.00  0.00           H
ATOM   1656 1HD2 LEU A 272     20.261  49.149   7.846  1.00  0.00           H
ATOM   1657 2HD2 LEU A 272     18.715  49.61 8   7.101  1.00  0.00           H
ATOM   1658 3HD2 LEU A 272     20.141  49.323   6.079  1.00  0.00           H
ATOM   1659  N   ALA A 273     18. 153  52. 102   3.083  1.00  0.00           N
ATOM   1660  CA  ALA A 273     17.450  52.796   2.019  1.00  0.00           C
ATOM   1661  C   ALA A 273     15.983  52.369   2.080  1.00  0.00           C
ATOM   1662  O   ALA A 273     15.703  5 1.253   2.5 19  1.00  0.00           O
ATOM   1663  CB  ALA A 273     18.065  52.389   0.678  1.00  0.00           C
ATOM   1664  H   ALA A 273     17.71 8  5 1.268   3.449  1.00  0.00           H
ATOM   1665  HA  ALA A 273     17.530  53.872   2. 171  1.00  0.00           H
ATOM   1666 1HB  ALA A 273     17.547  52.903  -0.13 1  1.00  0.00           H
ATOM   1667 2HB  ALA A 273     19.120  52.663   0.664  1.00  0.00           H
ATOM   1668 3HB  ALA A 273     17.969  5 1.3 12   0.545  1.00  0.00           H
ATOM   1669  N   PRO A 274     15.030  53.206   1.655  1.00  0.00           N
ATOM   1670  CA  PRO A 274     13.629  52.972   1.968  1.00  0.00           C
ATOM   1671  C   PRO A 274     13.037  5 1.885   1.076  1.00  0.00           C
ATOM   1672  O   PRO A 274     12.124  5 1.165   1.476  1.00  0.00           O
ATOM   1673  CB  PRO A 274     12.934  54.3 19   1.745  1.00  0.00           C
ATOM   1674  CG  PRO A 274     13.853  55.052   0.768  1.00  0.00           C
ATOM   1675  CD  PRO A 274     15.229  54.587   1.236  1.00  0.00           C
ATOM   1676  HA  PRO A 274     13.535  52.672   3.01 1  1.00  0.00           H
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ATOM   1677 1HB  PRO A 274      11.941  54.151   1.327  1.00  0.00           H
ATOM   1678 2HB  PRO A 274      12.844  54.844   2.696  1.00  0.00           H
ATOM   1679 1HG  PRO A 274      13.619  54.746  -0.252  1.00  0.00           H
ATOM   1680 2HG  PRO A 274      13.705  56.127   0.866  1.00  0.00           H
ATOM   1681 1HD  PRO A 274      15.589  55.175   2.081  1.00  0.00           H
ATOM   1682 2HD  PRO A 274      15.963  54.621   0.432  1.00  0.00           H
ATOM   1683  N   THR A 275      13.560  51.763  -0.140  1.00  0.00           N
ATOM   1684  CA  THR A 275      12.913  51.025  -1.200  1.00  0.00           C
ATOM   1685  C   THR A 275      13.906  50.045  -1.818  1.00  0.00           C
ATOM   1686  O   THR A 275      15.108  50.310  -1.898  1.00  0.00           O
ATOM   1687  CB  THR A 275      12.392  52.027  -2.241  1.00  0.00           C
ATOM   1688  CG2 THR A 275      11.259  52.880  -1.661  1.00  0.00           C
ATOM   1689  OG1 THR A 275      13.445  52.870  -2.668  1.00  0.00           O
ATOM   1690  H   THR A 275      14.446  52.198  -0.354  1.00  0.00           H
ATOM   1691  HA  THR A 275      12.046  50.499  -0.800  1.00  0.00           H
ATOM   1692  HB  THR A 275      12.032  51.487  -3.117  1.00  0.00           H
ATOM   1693 1HG2 THR A 275      10.907  53.581  -2.418  1.00  0.00           H
ATOM   1694 2HG2 THR A 275      10.436  52.233  -1.355  1.00  0.00           H
ATOM   1695 3HG2 THR A 275      11.626  53.433  -0.797  1.00  0.00           H
ATOM   1696  HG1 THR A 275      13.113  53.494  -3.318  1.00  0.00           H
ATOM   1697  N   ARG A 276      13.393  48.905  -2.292  1.00  0.00           N
ATOM   1698  CA  ARG A 276      14.191  47.935  -3.017  1.00  0.00           C
ATOM   1699  C   ARG A 276      14.982  48.614  -4.136  1.00  0.00           C
ATOM   1700  O   ARG A 276      16.090  48.191  -4.441  1.00  0.00           O
ATOM   1701  CB  ARG A 276      13.291  46.824  -3.584  1.00  0.00           C
ATOM   1702  CG  ARG A 276      14.081  45.908  -4.530  1.00  0.00           C
ATOM   1703  CD  ARG A 276      13.328  44.604  -4.820  1.00  0.00           C
ATOM   1704  NE  ARG A 276      13.890  43.843  -5.950  1.00  0.00           N
ATOM   1705  CZ  ARG A 276      15.146  43.455  -6.184  1.00  0.00           C
ATOM   1706  NH1 ARG A 276      16.072  43.621  -5.241  1.00  0.00           N1+
ATOM   1707  NH2 ARG A 276      15.481  42.919  -7.352  1.00  0.00           N
ATOM   1708  H   ARG A 276      12.416  48.693  -2.150  1.00  0.00           H
ATOM   1709  HA  ARG A 276      14.856  47.420  -2.324  1.00  0.00           H
ATOM   1710 1HB  ARG A 276      12.896  46.223  -2.764  1.00  0.00           H
ATOM   1711 2HB  ARG A 276      12.466  47.271  -4.137  1.00  0.00           H
ATOM   1712 1HG  ARG A 276      14.251  46.422  -5.476  1.00  0.00           H
ATOM   1713 2HG  ARG A 276      15.039  45.656  -4.077  1.00  0.00           H
ATOM   1714 1HD  ARG A 276      13.365  43.960  -3.942  1.00  0.00           H
ATOM   1715 2HD  ARG A 276      12.290  44.829  -5.062  1.00  0.00           H
ATOM   1716  HE  ARG A 276      13.160  43.613  -6.609  1.00  0.00           H
ATOM   1717 1HH1 ARG A 276      17.024  43.330  -5.410  1.00  0.00           H
ATOM   1718 2HH1 ARG A 276      15.821  44.038  -4.355  1.00  0.00           H
ATOM   1719 1HH2 ARG A 276      16.434  42.629  -7.520  1.00  0.00           H
ATOM   1720 2HH2 ARG A 276      14.783  42.802  -8.072  1.00  0.00           H
ATOM   1721  N   GLU A 277      14.393  49.613  -4.788  1.00  0.00           N
ATOM   1722  CA  GLU A 277      15.024  50.241  -5.924  1.00  0.00           C
ATOM   1723  C   GLU A 277      16.305  50.974  -5.517  1.00  0.00           C
ATOM   1724  O   GLU A 277      17.351  50.762  -6.127  1.00  0.00           O
ATOM   1725  CB  GLU A 277      14.053  51.204  -6.586  1.00  0.00           C
ATOM   1726  CG  GLU A 277      12.760  50.565  -7.095  1.00  0.00           C
ATOM   1727  CD  GLU A 277      12.041  51.522  -8.023  1.00  0.00           C
ATOM   1728  OE1 GLU A 277      12.337  52.732  -8.009  1.00  0.00           O
ATOM   1729  OE2 GLU A 277      11.172  51.061  -8.788  1.00  0.00           Ol-
ATOM   1730  H   GLU A 277      13.487  49.946  -4.491  1.00  0.00           H
ATOM   1731  HA  GLU A 277      15.240  49.488  -6.682  1.00  0.00           H
ATOM   1732 1HB  GLU A 277      13.762  51.975  -5.873  1.00  0.00           H
ATOM   1733 2HB  GLU A 277      14.533  51.669  -7.447  1.00  0.00           H
ATOM   1734 1HG  GLU A 277      12.995  49.649  -7.637  1.00  0.00           H
ATOM   1735 2HG  GLU A 277      12.113  50.330  -6.250  1.00  0.00           H
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ATOM 1736 N LEU A 278 16.224 51.868 -4.528 1.00 0.00 N
ATOM 1737 CA LEU A 278 17.405 52.612 -4.110 1.00 0.00 C
ATOM 1738 C LEU A 278 18.412 51.621 -3.526 1.00 0.00 C
ATOM 1739 O LEU A 278 19.616 51.735 -3.751 1.00 0.00 O
ATOM 1740 CB LEU A 278 17.038 53.724 -3.114 1.00 0.00 C
ATOM 1741 CG LEU A 278 18.201 54.695 -2.835 1.00 0.00 C
ATOM 1742 CD1 LEU A 278 18.479 55.613 -4.032 1.00 0.00 C
ATOM 1743 CD2 LEU A 278 17.866 55.582 -1.635 1.00 0.00 C
ATOM 1744 H LEU A 278 15.342 52.031 -4.065 1.00 0.00 H
ATOM 1745 HA LEU A 278 17.799 53.175 -4.956 1.00 0.00 H
ATOM 1746 1HB LEU A 278 16.208 54.309 -3.511 1.00 0.00 H
ATOM 1747 2HB LEU A 278 16.746 53.279 -2.163 1.00 0.00 H
ATOM 1748 HG LEU A 278 19.108 54.127 -2.628 1.00 0.00 H
ATOM 1749 1HD1 LEU A 278 19.306 56.282 -3.793 1.00 0.00 H
ATOM 1750 2HD1 LEU A 278 18.740 55.009 -4.901 1.00 0.00 H
ATOM 1751 3HD1 LEU A 278 17.588 56.202 -4.253 1.00 0.00 H
ATOM 1752 1HD2 LEU A 278 18.694 56.266 -1.445 1.00 0.00 H
ATOM 1753 2HD2 LEU A 278 16.964 56.155 -1.846 1.00 0.00 H
ATOM 1754 3HD2 LEU A 278 17.702 54.958 -0.756 1.00 0.00 H
ATOM 1755 N ALA A 279 17.910 50.622 -2.794 1.00 0.00 N
ATOM 1756 CA ALA A 279 18.759 49.596 -2.224 1.00 0.00 C
ATOM 1757 C ALA A 279 19.503 48.828 -3.324 1.00 0.00 C
ATOM 1758 O ALA A 279 20.635 48.391 -3.125 1.00 0.00 O
ATOM 1759 CB ALA A 279 17.927 48.651 -1.353 1.00 0.00 C
ATOM 1760 H ALA A 279 16.915 50.570 -2.626 1.00 0.00 H
ATOM 1761 HA ALA A 279 19.450 50.049 -1.513 1.00 0.00 H
ATOM 1762 1HB ALA A 279 18.574 47.883 -0.929 1.00 0.00 H
ATOM 1763 2HB ALA A 279 17.459 49.216 -0.547 1.00 0.00 H
ATOM 1764 3HB ALA A 279 17.155 48.180 -1.961 1.00 0.00 H
ATOM 1765 N VAL A 280 18.854 48.620 -4.470 1.00 0.00 N
ATOM 1766 CA VAL A 280 19.473 48.004 -5.628 1.00 0.00 C
ATOM 1767 C VAL A 280 20.518 48.956 -6.208 1.00 0.00 C
ATOM 1768 O VAL A 280 21.645 48.516 -6.421 1.00 0.00 O
ATOM 1769 CB VAL A 280 18.407 47.539 -6.640 1.00 0.00 C
ATOM 1770 CGI VAL A 280 18.967 47.287 -8.046 1.00 0.00 C
ATOM 1771 CG2 VAL A 280 17.779 46.224 -6.157 1.00 0.00 C
ATOM 1772 H VAL A 280 17.886 48.895 -4.559 1.00 0.00 H
ATOM 1773 HA VAL A 280 19.847 47.016 -5.358 1.00 0.00 H
ATOM 1774 HB VAL A 280 17.633 48.301 -6.731 1.00 0.00 H
ATOM 1775 1HG1 VAL A 280 18.162 46.962 -8.706 1.00 0.00 H
ATOM 1776 2HG1 VAL A 280 19.405 48.207 -8.434 1.00 0.00 H
ATOM 1777 3HG1 VAL A 280 19.733 46.512 -8.000 1.00 0.00 H
ATOM 1778 1HG2 VAL A 280 17.026 45.895 -6.873 1.00 0.00 H
ATOM 1779 2HG2 VAL A 280 18.553 45.461 -6.069 1.00 0.00 H
ATOM 1780 3HG2 VAL A 280 17.311 46.380 -5.184 1.00 0.00 H
ATOM 1781 N GLN A 281 20.166 50.224 -6.472 1.00 0.00 N
ATOM 1782 CA GLN A 281 21.088 51.189 -7.071 1.00 0.00 C
ATOM 1783 C GLN A 281 22.471 51.080 -6.439 1.00 0.00 C
ATOM 1784 O GLN A 281 23.470 50.881 -7.122 1.00 0.00 O
ATOM 1785 CB GLN A 281 20.627 52.645 -6.899 1.00 0.00 C
ATOM 1786 CG GLN A 281 19.431 53.044 -7.762 1.00 0.00 C
ATOM 1787 CD GLN A 281 19.547 54.513 -8.153 1.00 0.00 C
ATOM 1788 NE2 GLN A 281 18.725 55.397 -7.602 1.00 0.00 N
ATOM 1789 OE1 GLN A 281 20.404 54.871 -8.948 1.00 0.00 O
ATOM 1790 H GLN A 281 19.233 50.544 -6.255 1.00 0.00 H
ATOM 1791 HA GLN A 281 21.172 50.996 -8.140 1.00 0.00 H
ATOM 1792 1HB GLN A 281 20.336 52.814 -5.863 1.00 0.00 H
ATOM 1793 2HB GLN A 281 21.442 53.318 -7.162 1.00 0.00 H
ATOM 1794 1HG GLN A 281 19.412 52.431 -8.664 1.00 0.00 H

ATOM 1795 2HG GLN A 281 18.509 52.891 -7.200 1.00 0.00 H
ATOM 1796 1HE2 GLN A 281 18.792 56.373 -7.853 1.00 0.00 H
ATOM 1797 2HE2 GLN A 281 18.033 55.094 -6.932 1.00 0.00 H
ATOM 1798 N ILE A 282 22.509 51.243 -5.122 1.00 0.00 N
ATOM 1799 CA ILE A 282 23.742 51.381 -4.374 1.00 0.00 C
ATOM 1800 C ILE A 282 24.575 50.098 -4.512 1.00 0.00 C
ATOM 1801 O ILE A 282 25.804 50.132 -4.476 1.00 0.00 O
ATOM 1802 CB ILE A 282 23.368 51.706 -2.917 1.00 0.00 C
ATOM 1803 CGI ILE A 282 22.624 53.055 -2.844 1.00 0.00 C
ATOM 1804 CG2 ILE A 282 24.610 51.754 -2.022 1.00 0.00 C
ATOM 1805 CD1 ILE A 282 21.823 53.232 -1.551 1.00 0.00 C
ATOM 1806 H ILE A 282 21.650 51.277 -4.592 1.00 0.00 H
ATOM 1807 HA ILE A 282 24.283 52.261 -4.723 1.00 0.00 H
ATOM 1808 HB ILE A 282 22.750 50.904 -2.512 1.00 0.00 H
ATOM 1809 1HG1 ILE A 282 23.344 53.872 -2.900 1.00 0.00 H
ATOM 1810 2HG1 ILE A 282 21.925 53.131 -3.677 1.00 0.00 H
ATOM 1811 1HG2 ILE A 282 24.313 51.985 -0.999 1.00 0.00 H
ATOM 1812 2HG2 ILE A 282 25.112 50.786 -2.044 1.00 0.00 H
ATOM 1813 3HG2 ILE A 282 25.291 52.524 -2.385 1.00 0.00 H
ATOM 1814 1HD1 ILE A 282 21.324 54.201 -1.562 1.00 0.00 H
ATOM 1815 2HD1 ILE A 282 21.078 52.440 -1.473 1.00 0.00 H
ATOM 1816 3HD1 ILE A 282 22.498 53.181 -0.696 1.00 0.00 H
ATOM 1817 N TYR A 283 23.908 48.955 -4.642 1.00 0.00 N
ATOM 1818 CA TYR A 283 24.547 47.658 -4.729 1.00 0.00 C
ATOM 1819 C TYR A 283 25.065 47.413 -6.149 1.00 0.00 C
ATOM 1820 O TYR A 283 26.177 46.906 -6.320 1.00 0.00 O
ATOM 1821 CB TYR A 283 23.558 46.587 -4.255 1.00 0.00 C
ATOM 1822 CG TYR A 283 23.778 45.198 -4.819 1.00 0.00 C
ATOM 1823 CD1 TYR A 283 24.805 44.368 -4.335 1.00 0.00 C
ATOM 1824 CD2 TYR A 283 22.946 44.722 -5.846 1.00 0.00 C
ATOM 1825 CE1 TYR A 283 25.002 43.088 -4.882 1.00 0.00 C
ATOM 1826 CE2 TYR A 283 23.122 43.435 -6.373 1.00 0.00 C
ATOM 1827 CZ TYR A 283 24.165 42.612 -5.909 1.00 0.00 C
ATOM 1828 OH TYR A 283 24.367 41.377 -6.453 1.00 0.00 O
ATOM 1829 H TYR A 283 22.899 48.962 -4.686 1.00 0.00 H
ATOM 1830 HA TYR A 283 25.331 47.588 -3.976 1.00 0.00 H
ATOM 1831 1HB TYR A 283 23.618 46.491 -3.171 1.00 0.00 H
ATOM 1832 2HB TYR A 283 22.545 46.876 -4.538 1.00 0.00 H
ATOM 1833 HD1 TYR A 283 25.448 44.712 -3.539 1.00 0.00 H
ATOM 1834 HD2 TYR A 283 22.160 45.349 -6.240 1.00 0.00 H
ATOM 1835 HE1 TYR A 283 25.801 42.461 -4.515 1.00 0.00 H
ATOM 1836 HE2 TYR A 283 22.455 43.069 -7.139 1.00 0.00 H
ATOM 1837 HH TYR A 283 23.710 41.216 -7.135 1.00 0.00 H
ATOM 1838 N GLU A 284 24.262 47.743 -7.161 1.00 0.00 N
ATOM 1839 CA GLU A 284 24.687 47.674 -8.547 1.00 0.00 C
ATOM 1840 C GLU A 284 25.887 48.609 -8.743 1.00 0.00 C
ATOM 1841 O GLU A 284 26.858 48.246 -9.408 1.00 0.00 O
ATOM 1842 CB GLU A 284 23.527 48.053 -9.481 1.00 0.00 C
ATOM 1843 CG GLU A 284 22.327 47.093 -9.389 1.00 0.00 C
ATOM 1844 CD GLU A 284 22.666 45.688 -9.839 1.00 0.00 C
ATOM 1845 OE1 GLU A 284 22.332 44.727 -9.116 1.00 0.00 O
ATOM 1846 OE2 GLU A 284 23.365 45.544 -10.861 1.00 0.00 Ol-
ATOM 1847 H GLU A 284 23.319 48.055 -6.977 1.00 0.00 H
ATOM 1848 HA GLU A 284 24.932 46.643 -8.802 1.00 0.00 H
ATOM 1849 1HB GLU A 284 23.167 49.050 -9.227 1.00 0.00 H
ATOM 1850 2HB GLU A 284 23.874 48.044 -10.514 1.00 0.00 H
ATOM 1851 IHG GLU A 284 21.984 47.038 -8.356 1.00 0.00 H
ATOM 1852 2HG GLU A 284 21.519 47.460 -10.021 1.00 0.00 H
ATOM 1853 N GLU A 285 25.808 49.804 -8.157 1.00 0.00 N

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ATOM   1854  CA  GLU A 285      26.842  50.816  -8.227  1.00  0.00           C
ATOM   1855  C   GLU A 285      28.108  50.279  -7.558  1.00  0.00           C
ATOM   1856  O   GLU A 285      29.181  50.265  -8.161  1.00  0.00           O
ATOM   1857  CB  GLU A 285      26.347  52.107  -7.554  1.00  0.00           C
ATOM   1858  CG  GLU A 285      27.281  53.309  -7.766  1.00  0.00           C
ATOM   1859  CD  GLU A 285      27.335  53.738  -9.217  1.00  0.00           C
ATOM   1860  OE1 GLU A 285      26.439  53.347  -9.990  1.00  0.00           O
ATOM   1861  OE2 GLU A 285      28.310  54.402  -9.628  1.00  0.00           Ol-
ATOM   1862  H   GLU A 285      24.987  50.052  -7.623  1.00  0.00           H
ATOM   1863  HA  GLU A 285      27.018  51.085  -9.268  1.00  0.00           H
ATOM   1864 1HB  GLU A 285      25.372  52.378  -7.959  1.00  0.00           H
ATOM   1865 2HB  GLU A 285      26.262  51.948  -6.479  1.00  0.00           H
ATOM   1866 1HG  GLU A 285      26.927  54.154  -7.175  1.00  0.00           H
ATOM   1867 2HG  GLU A 285      28.291  53.045  -7.452  1.00  0.00           H
ATOM   1868  N   ALA A 286      28.000  49.850  -6.298  1.00  0.00           N
ATOM   1869  CA  ALA A 286      29.146  49.426  -5.512  1.00  0.00           C
ATOM   1870  C   ALA A 286      29.958  48.357  -6.240  1.00  0.00           C
ATOM   1871  O   ALA A 286      31.179  48.307  -6.101  1.00  0.00           O
ATOM   1872  CB  ALA A 286      28.691  48.907  -4.146  1.00  0.00           C
ATOM   1873  H   ALA A 286      27.093  49.811  -5.854  1.00  0.00           H
ATOM   1874  HA  ALA A 286      29.768  50.290  -5.280  1.00  0.00           H
ATOM   1875 1HB  ALA A 286      29.560  48.592  -3.568  1.00  0.00           H
ATOM   1876 2HB  ALA A 286      28.167  49.699  -3.612  1.00  0.00           H
ATOM   1877 3HB  ALA A 286      28.021  48.058  -4.285  1.00  0.00           H
ATOM   1878  N   ARG A 287      29.284  47.487  -6.992  1.00  0.00           N
ATOM   1879  CA  ARG A 287      29.925  46.416  -7.735  1.00  0.00           C
ATOM   1880  C   ARG A 287      30.885  46.924  -8.812  1.00  0.00           C
ATOM   1881  O   ARG A 287      31.715  46.147  -9.278  1.00  0.00           O
ATOM   1882  CB  ARG A 287      28.863  45.507  -8.352  1.00  0.00           C
ATOM   1883  CG  ARG A 287      28.356  44.488  -7.323  1.00  0.00           C
ATOM   1884  CD  ARG A 287      27.022  43.862  -7.742  1.00  0.00           C
ATOM   1885  NE  ARG A 287      26.890  43.746  -9.207  1.00  0.00           N
ATOM   1886  CZ  ARG A 287      25.700  43.825  -9.812  1.00  0.00           C
ATOM   1887  NH1 ARG A 287      24.626  43.448  -9.131  1.00  0.00           N1+
ATOM   1888  NH2 ARG A 287      25.609  44.283 -11.055  1.00  0.00           N
ATOM   1889  H   ARG A 287      28.279  47.555  -7.065  1.00  0.00           H
ATOM   1890  HA  ARG A 287      30.441  45.751  -7.042  1.00  0.00           H
ATOM   1891 1HB  ARG A 287      28.021  46.110  -8.693  1.00  0.00           H
ATOM   1892 2HB  ARG A 287      29.291  44.970  -9.198  1.00  0.00           H
ATOM   1893 1HG  ARG A 287      29.087  43.687  -7.214  1.00  0.00           H
ATOM   1894 2HG  ARG A 287      28.212  44.982  -6.362  1.00  0.00           H
ATOM   1895 1HD  ARG A 287      26.940  42.861  -7.317  1.00  0.00           H
ATOM   1896 2HD  ARG A 287      26.200  44.478  -7.379  1.00  0.00           H
ATOM   1897  HE  ARG A 287      27.726  43.604  -9.754  1.00  0.00           H
ATOM   1898 1HH1 ARG A 287      23.713  43.496  -9.561  1.00  0.00           H
ATOM   1899 2HH1 ARG A 287      24.721  43.113  -8.183  1.00  0.00           H
ATOM   1900 1HH2 ARG A 287      24.708  44.341 -11.508  1.00  0.00           H
ATOM   1901 2HH2 ARG A 287      26.442  44.573 -11.548  1.00  0.00           H
ATOM   1902  N   LYS A 288      30.781  48.184  -9.234  1.00  0.00           N
ATOM   1903  CA  LYS A 288      31.797  48.774 -10.091  1.00  0.00           C
ATOM   1904  C   LYS A 288      33.121  48.769  -9.329  1.00  0.00           C
ATOM   1905  O   LYS A 288      34.162  48.375  -9.845  1.00  0.00           O
ATOM   1906  CB  LYS A 288      31.424  50.221 -10.439  1.00  0.00           C
ATOM   1907  CG  LYS A 288      30.187  50.349 -11.338  1.00  0.00           C
ATOM   1908  CD  LYS A 288      29.610  51.763 -11.182  1.00  0.00           C
ATOM   1909  CE  LYS A 288      28.734  52.170 -12.374  1.00  0.00           C
ATOM   1910  NZ  LYS A 288      27.943  53.375 -12.066  1.00  0.00           N1+
ATOM   1911  H   LYS A 288      29.988  48.745  -8.959  1.00  0.00           H
ATOM   1912  HA  LYS A 288      31.899  48.177 -10.998  1.00  0.00           H
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ATOM 1913 1HB LYS A 288 31.213 50.773 -9.523 1.00 0.00 H
ATOM 1914 2HB LYS A 288 32.253 50.694 -10.965 1.00 0.00 H
ATOM 1915 1HG LYS A 288 30.472 50.177 -12.376 1.00 0.00 H
ATOM 1916 2HG LYS A 288 29.443 49.610 -11.039 1.00 0.00 H
ATOM 1917 IHD LYS A 288 28.997 51.809 -10.282 1.00 0.00 H
ATOM 1918 2HD LYS A 288 30.426 52.481 -11.103 1.00 0.00 H
ATOM 1919 1HE LYS A 288 29.367 52.380 -13.236 1.00 0.00 H
ATOM 1920 2HE LYS A 288 28.049 51.357 -12.616 1.00 0.00 H
ATOM 1921 1HZ LYS A 288 27.377 53.620 -12.866 1.00 0.00 H
ATOM 1922 2HZ LYS A 288 27.345 53.192 -11.274 1.00 0.00 H
ATOM 1923 3HZ LYS A 288 28.566 54.140 -11.848 1.00 0.00 H
ATOM 1924 N PHE A 289 33.076 49.243 -8.087 1.00 0.00 N
ATOM 1925 CA PHE A 289 34.248 49.704 -7.368 1.00 0.00 C
ATOM 1926 C PHE A 289 34.636 48.717 -6.272 1.00 0.00 C
ATOM 1927 O PHE A 289 35.463 49.028 -5.418 1.00 0.00 O
ATOM 1928 CB PHE A 289 33.965 51.104 -6.817 1.00 0.00 C
ATOM 1929 CG PHE A 289 33.732 52.146 -7.893 1.00 0.00 C
ATOM 1930 CDl PHE A 289 34.785 52.507 -8.753 1.00 0.00 C
ATOM 1931 CD2 PHE A 289 32.475 52.760 -8.058 1.00 0.00 C
ATOM 1932 CE1 PHE A 289 34.597 53.466 -9.760 1.00 0.00 C
ATOM 1933 CE2 PHE A 289 32.280 53.722 -9.065 1.00 0.00 C
ATOM 1934 CZ PHE A 289 33.343 54.078 -9.913 1.00 0.00 C
ATOM 1935 H PHE A 289 32.193 49.296 -7.598 1.00 0.00 H
ATOM 1936 HA PHE A 289 35.064 49.871 -8.072 1.00 0.00 H
ATOM 1937 1HB PHE A 289 33.071 51.076 -6.194 1.00 0.00 H
ATOM 1938 2HB PHE A 289 34.814 51.439 -6.220 1.00 0.00 H
ATOM 1939 HDl PHE A 289 35.755 52.044 -8.644 1.00 0.00 H
ATOM 1940 HD2 PHE A 289 31.654 52.493 -7.410 1.00 0.00 H
ATOM 1941 HE1 PHE A 289 35.415 53.731 -10.414 1.00 0.00 H
ATOM 1942 HE2 PHE A 289 31.312 54.187 -9.187 1.00 0.00 H
ATOM 1943 HZ PHE A 289 33.196 54.823 -10.681 1.00 0.00 H
ATOM 1944 N SER A 290 34.052 47.521 -6.303 1.00 0.00 N
ATOM 1945 CA SER A 290 34.524 46.369 -5.552 1.00 0.00 C
ATOM 1946 C SER A 290 34.973 45.280 -6.531 1.00 0.00 C
ATOM 1947 O SER A 290 35.242 44.144 -6.141 1.00 0.00 O
ATOM 1948 CB SER A 290 33.426 45.887 -4.595 1.00 0.00 C
ATOM 1949 OG SER A 290 32.132 45.976 -5.162 1.00 0.00 O
ATOM 1950 H SER A 290 33.231 47.374 -6.873 1.00 0.00 H
ATOM 1951 HA SER A 290 35.317 46.678 -4.871 1.00 0.00 H
ATOM 1952 1HB SER A 290 33.605 44.845 -4.331 1.00 0.00 H
ATOM 1953 2HB SER A 290 33.438 46.497 -3.692 1.00 0.00 H
ATOM 1954 HG SER A 290 31.482 45.665 -4.527 1.00 0.00 H
ATOM 1955 N TYR A 291 35.055 45.616 -7.820 1.00 0.00 N
ATOM 1956 CA TYR A 291 35.599 44.690 -8.784 1.00 0.00 C
ATOM 1957 C TYR A 291 37.116 44.707 -8.598 1.00 0.00 C
ATOM 1958 O TYR A 291 37.768 45.699 -8.927 1.00 0.00 O
ATOM 1959 CB TYR A 291 35.168 45.073 -10.206 1.00 0.00 C
ATOM 1960 CG TYR A 291 35.644 44.108 -11.278 1.00 0.00 C
ATOM 1961 CDl TYR A 291 35.248 42.757 -11.250 1.00 0.00 C
ATOM 1962 CD2 TYR A 291 36.486 44.539 -12.320 1.00 0.00 C
ATOM 1963 CE1 TYR A 291 35.698 41.857 -12.231 1.00 0.00 C
ATOM 1964 CE2 TYR A 291 36.930 43.643 -13.306 1.00 0.00 C
ATOM 1965 CZ TYR A 291 36.543 42.291 -13.266 1.00 0.00 C
ATOM 1966 OH TYR A 291 36.970 41.407 -14.216 1.00 0.00 O
ATOM 1967 H TYR A 291 34.736 46.523 -8.127 1.00 0.00 H
ATOM 1968 HA TYR A 291 35.154 43.706 -8.636 1.00 0.00 H
ATOM 1969 1HB TYR A 291 34.079 45.101 -10.260 1.00 0.00 H
ATOM 1970 2HB TYR A 291 35.570 46.055 -10.456 1.00 0.00 H
ATOM 1971 HDl TYR A 291 34.593 42.403 -10.468 1.00 0.00 H

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ATOM   1972  HD2 TYR A 291      36.801  45.571 -12.369  1.00  0.00           H
ATOM   1973  HE1 TYR A 291      35.393  40.821 -12.193  1.00  0.00           H
ATOM   1974  HE2 TYR A 291      37.571  43.990 -14.103  1.00  0.00           H
ATOM   1975  HH  TYR A 291      37.536  41.861 -14.845  1.00  0.00           H
ATOM   1976  N   ARG A 292      37.658  43.601  -8.077  1.00  0.00           N
ATOM   1977  CA  ARG A 292      39.075  43.308  -7.892  1.00  0.00           C
ATOM   1978  C   ARG A 292      39.546  43.710  -6.486  1.00  0.00           C
ATOM   1979  O   ARG A 292      40.662  44.200  -6.338  1.00  0.00           O
ATOM   1980  CB  ARG A 292      39.976  43.919  -8.987  1.00  0.00           C
ATOM   1981  CG  ARG A 292      39.522  43.636 -10.435  1.00  0.00           C
ATOM   1982  CD  ARG A 292      40.123  44.654 -11.414  1.00  0.00           C
ATOM   1983  NE  ARG A 292      39.767  46.042 -11.053  1.00  0.00           N
ATOM   1984  CZ  ARG A 292      40.600  47.083 -11.222  1.00  0.00           C
ATOM   1985  NH1 ARG A 292      41.584  46.972 -12.107  1.00  0.00           N1+
ATOM   1986  NH2 ARG A 292      40.469  48.185 -10.489  1.00  0.00           N
ATOM   1987  H   ARG A 292      37.063  42.849  -7.758  1.00  0.00           H
ATOM   1988  HA  ARG A 292      39.266  42.263  -8.137  1.00  0.00           H
ATOM   1989  1HB ARG A 292      40.002  45.003  -8.873  1.00  0.00           H
ATOM   1990  2HB ARG A 292      40.986  43.520  -8.892  1.00  0.00           H
ATOM   1991  1HG ARG A 292      39.845  42.638 -10.729  1.00  0.00           H
ATOM   1992  2HG ARG A 292      38.435  43.697 -10.494  1.00  0.00           H
ATOM   1993  1HD ARG A 292      41.209  44.567 -11.407  1.00  0.00           H
ATOM   1994  2HD ARG A 292      39.750  44.456 -12.419  1.00  0.00           H
ATOM   1995  HE  ARG A 292      38.848  46.189 -10.662  1.00  0.00           H
ATOM   1996  1HH1 ARG A 292      42.222  47.741 -12.252  1.00  0.00           H
ATOM   1997  2HH1 ARG A 292      41.694  46.118 -12.636  1.00  0.00           H
ATOM   1998  1HH2 ARG A 292      41.101  48.960 -10.626  1.00  0.00           H
ATOM   1999  2HH2 ARG A 292      39.738  48.246  -9.795  1.00  0.00           H
ATOM   2000  N   SER A 293      38.755  43.475  -5.434  1.00  0.00           N
ATOM   2001  CA  SER A 293      39.187  43.837  -4.091  1.00  0.00           C
ATOM   2002  C   SER A 293      38.512  42.970  -3.020  1.00  0.00           C
ATOM   2003  O   SER A 293      37.691  42.108  -3.330  1.00  0.00           O
ATOM   2004  CB  SER A 293      38.928  45.332  -3.870  1.00  0.00           C
ATOM   2005  OG  SER A 293      37.542  45.609  -3.784  1.00  0.00           O
ATOM   2006  H   SER A 293      37.852  43.043  -5.568  1.00  0.00           H
ATOM   2007  HA  SER A 293      40.274  43.783  -4.031  1.00  0.00           H
ATOM   2008  1HB SER A 293      39.402  45.650  -2.941  1.00  0.00           H
ATOM   2009  2HB SER A 293      39.343  45.900  -4.702  1.00  0.00           H
ATOM   2010  HG  SER A 293      37.411  46.550  -3.646  1.00  0.00           H
ATOM   2011  N   ARG A 294      38.852  43.181  -1.741  1.00  0.00           N
ATOM   2012  CA  ARG A 294      38.394  42.338  -0.641  1.00  0.00           C
ATOM   2013  C   ARG A 294      36.948  42.658  -0.229  1.00  0.00           C
ATOM   2014  O   ARG A 294      36.636  42.720   0.961  1.00  0.00           O
ATOM   2015  CB  ARG A 294      39.363  42.451   0.556  1.00  0.00           C
ATOM   2016  CG  ARG A 294      39.528  43.875   1.128  1.00  0.00           C
ATOM   2017  CD  ARG A 294      40.010  43.824   2.588  1.00  0.00           C
ATOM   2018  NE  ARG A 294      40.237  45.172   3.144  1.00  0.00           N
ATOM   2019  CZ  ARG A 294      40.343  45.502   4.442  1.00  0.00           C
ATOM   2020  NH1 ARG A 294      40.181  44.572   5.383  1.00  0.00           N1+
ATOM   2021  NH2 ARG A 294      40.597  46.761   4.788  1.00  0.00           N
ATOM   2022  H   ARG A 294      39.455  43.955  -1.500  1.00  0.00           H
ATOM   2023  HA  ARG A 294      38.519  41.289  -0.909  1.00  0.00           H
ATOM   2024  1HB ARG A 294      39.005  41.826   1.374  1.00  0.00           H
ATOM   2025  2HB ARG A 294      40.356  42.119   0.253  1.00  0.00           H
ATOM   2026  1HG ARG A 294      40.260  44.423   0.534  1.00  0.00           H
ATOM   2027  2HG ARG A 294      38.570  44.395   1.092  1.00  0.00           H
ATOM   2028  1HD ARG A 294      39.260  43.325   3.202  1.00  0.00           H
ATOM   2029  2HD ARG A 294      40.949  43.271   2.642  1.00  0.00           H
ATOM   2030  HE  ARG A 294      40.315  45.887   2.434  1.00  0.00           H
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ATOM   2031 1HH1 ARG A 294     40.261  44.822   6.359  1.00  0.00           H
ATOM   2032 2HH1 ARG A 294     39.979  43.618   5.122  1.00  0.00           H
ATOM   2033 1HH2 ARG A 294     40.677  47.010   5.763  1.00  0.00           H
ATOM   2034 2HH2 ARG A 294     40.711  47.467   4.075  1.00  0.00           H
ATOM   2035  N   VAL A 295     36.046  42.852  -1.188  1.00  0.00           N
ATOM   2036  CA  VAL A 295     34.715  43.379  -0.946  1.00  0.00           C
ATOM   2037  C   VAL A 295     33.719  42.549  -1.752  1.00  0.00           C
ATOM   2038  O   VAL A 295     33.739  42.568  -2.976  1.00  0.00           O
ATOM   2039  CB  VAL A 295     34.663  44.867  -1.339  1.00  0.00           C
ATOM   2040  CGI VAL A 295     33.277  45.455  -1.033  1.00  0.00           C
ATOM   2041  CG2 VAL A 295     35.716  45.682  -0.581  1.00  0.00           C
ATOM   2042  H   VAL A 295     36.272  42.628  -2.147  1.00  0.00           H
ATOM   2043  HA  VAL A 295     34.499  43.346   0.122  1.00  0.00           H
ATOM   2044  HB  VAL A 295     34.875  44.970  -2.403  1.00  0.00           H
ATOM   2045 1HG1 VAL A 295     33.258  46.507  -1.316  1.00  0.00           H
ATOM   2046 2HG1 VAL A 295     32.519  44.913  -1.598  1.00  0.00           H
ATOM   2047 3HG1 VAL A 295     33.070  45.363   0.034  1.00  0.00           H
ATOM   2048 1HG2 VAL A 295     35.652  46.728  -0.881  1.00  0.00           H
ATOM   2049 2HG2 VAL A 295     35.536  45.601   0.491  1.00  0.00           H
ATOM   2050 3HG2 VAL A 295     36.709  45.298  -0.812  1.00  0.00           H
ATOM   2051  N   ARG A 296     32.823  41.844  -1.063  1.00  0.00           N
ATOM   2052  CA  ARG A 296     31.770  41.061  -1.682  1.00  0.00           C
ATOM   2053  C   ARG A 296     30.447  41.647  -1.182  1.00  0.00           C
ATOM   2054  O   ARG A 296     30.099  41.440  -0.016  1.00  0.00           O
ATOM   2055  CB  ARG A 296     31.966  39.590  -1.290  1.00  0.00           C
ATOM   2056  CG  ARG A 296     30.994  38.616  -1.977  1.00  0.00           C
ATOM   2057  CD  ARG A 296     29.710  38.347  -1.173  1.00  0.00           C
ATOM   2058  NE  ARG A 296     28.509  38.973  -1.761  1.00  0.00           N
ATOM   2059  CZ  ARG A 296     27.307  38.380  -1.874  1.00  0.00           C
ATOM   2060  NH1 ARG A 296     27.047  37.241  -1.241  1.00  0.00           N1+
ATOM   2061  NH2 ARG A 296     26.381  38.943  -2.637  1.00  0.00           N
ATOM   2062  H   ARG A 296     32.854  41.836  -0.053  1.00  0.00           H
ATOM   2063  HA  ARG A 296     31.869  41.112  -2.767  1.00  0.00           H
ATOM   2064 1HB  ARG A 296     32.974  39.274  -1.556  1.00  0.00           H
ATOM   2065 2HB  ARG A 296     31.822  39.478  -0.216  1.00  0.00           H
ATOM   2066 1HG  ARG A 296     30.691  39.023  -2.942  1.00  0.00           H
ATOM   2067 2HG  ARG A 296     31.487  37.655  -2.127  1.00  0.00           H
ATOM   2068 1HD  ARG A 296     29.529  37.273  -1.125  1.00  0.00           H
ATOM   2069 2HD  ARG A 296     29.823  38.742  -0.164  1.00  0.00           H
ATOM   2070  HE  ARG A 296     28.639  39.918  -2.092  1.00  0.00           H
ATOM   2071 1HH1 ARG A 296     26.140  36.807  -1.335  1.00  0.00           H
ATOM   2072 2HH1 ARG A 296     27.756  36.810  -0.665  1.00  0.00           H
ATOM   2073 1HH2 ARG A 296     25.473  38.510  -2.732  1.00  0.00           H
ATOM   2074 2HH2 ARG A 296     26.582  39.805  -3.124  1.00  0.00           H
ATOM   2075  N   PRO A 297     29.714  42.390  -2.026  1.00  0.00           N
ATOM   2076  CA  PRO A 297     28.584  43.196  -1.573  1.00  0.00           C
ATOM   2077  C   PRO A 297     27.278  42.423  -1.798  1.00  0.00           C
ATOM   2078  O   PRO A 297     27.277  41.414  -2.507  1.00  0.00           O
ATOM   2079  CB  PRO A 297     28.634  44.468  -2.421  1.00  0.00           C
ATOM   2080  CG  PRO A 297     29.207  43.973  -3.746  1.00  0.00           C
ATOM   2081  CD  PRO A 297     30.214  42.917  -3.294  1.00  0.00           C
ATOM   2082  HA  PRO A 297     28.695  43.414  -0.511  1.00  0.00           H
ATOM   2083 1HB  PRO A 297     27.629  44.875  -2.526  1.00  0.00           H
ATOM   2084 2HB  PRO A 297     29.275  45.204  -1.936  1.00  0.00           H
ATOM   2085 1HG  PRO A 297     28.405  43.559  -4.357  1.00  0.00           H
ATOM   2086 2HG  PRO A 297     29.673  44.804  -4.274  1.00  0.00           H
ATOM   2087 1HD  PRO A 297     31.200  43.356  -3.141  1.00  0.00           H
ATOM   2088 2HD  PRO A 297     30.286  42.108  -4.021  1.00  0.00           H
ATOM   2089  N   CYS A 298     26.169  42.871  -1.210  1.00  0.00           N
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ATOM   2090  CA  CYS A 298      24.891  42.167  -1.192  1.00  0.00           C
ATOM   2091  C   CYS A 298      23.780  43.197  -0.971  1.00  0.00           C
ATOM   2092  O   CYS A 298      24.037  44.242  -0.374  1.00  0.00           O
ATOM   2093  CB  CYS A 298      24.924  41.140  -0.049  1.00  0.00           C
ATOM   2094  SG  CYS A 298      23.385  40.185   0.073  1.00  0.00           S
ATOM   2095  H   CYS A 298      26.176  43.761  -0.733  1.00  0.00           H
ATOM   2096  HA  CYS A 298      24.746  41.651  -2.142  1.00  0.00           H
ATOM   2097  1HB CYS A 298      25.741  40.439  -0.213  1.00  0.00           H
ATOM   2098  2HB CYS A 298      25.073  41.657   0.899  1.00  0.00           H
ATOM   2099  HG  CYS A 298      23.463  39.468   0.904  1.00  0.00           H
ATOM   2100  N   VAL A 299      22.560  42.899  -1.422  1.00  0.00           N
ATOM   2101  CA  VAL A 299      21.386  43.734  -1.217  1.00  0.00           C
ATOM   2102  C   VAL A 299      20.258  42.838  -0.706  1.00  0.00           C
ATOM   2103  O   VAL A 299      20.076  41.732  -1.219  1.00  0.00           O
ATOM   2104  CB  VAL A 299      21.004  44.459  -2.521  1.00  0.00           C
ATOM   2105  CGI VAL A 299      20.693  43.513  -3.689  1.00  0.00           C
ATOM   2106  CG2 VAL A 299      19.814  45.400  -2.300  1.00  0.00           C
ATOM   2107  H   VAL A 299      22.408  42.047  -1.942  1.00  0.00           H
ATOM   2108  HA  VAL A 299      21.629  44.539  -0.524  1.00  0.00           H
ATOM   2109  HB  VAL A 299      21.797  45.153  -2.797  1.00  0.00           H
ATOM   2110  1HG1 VAL A 299      20.432  44.098  -4.571  1.00  0.00           H
ATOM   2111  2HG1 VAL A 299      21.569  42.901  -3.905  1.00  0.00           H
ATOM   2112  3HG1 VAL A 299      19.857  42.867  -3.422  1.00  0.00           H
ATOM   2113  1HG2 VAL A 299      19.566  45.898  -3.237  1.00  0.00           H
ATOM   2114  2HG2 VAL A 299      18.955  44.825  -1.956  1.00  0.00           H
ATOM   2115  3HG2 VAL A 299      20.076  46.147  -1.550  1.00  0.00           H
ATOM   2116  N   VAL A 300      19.497  43.303   0.284  1.00  0.00           N
ATOM   2117  CA  VAL A 300      18.382  42.565   0.860  1.00  0.00           C
ATOM   2118  C   VAL A 300      17.181  43.503   0.983  1.00  0.00           C
ATOM   2119  O   VAL A 300      17.339  44.702   1.194  1.00  0.00           O
ATOM   2120  CB  VAL A 300      18.782  41.913   2.195  1.00  0.00           C
ATOM   2121  CGI VAL A 300      19.962  40.955   1.985  1.00  0.00           C
ATOM   2122  CG2 VAL A 300      19.134  42.937   3.280  1.00  0.00           C
ATOM   2123  H   VAL A 300      19.682  44.214   0.677  1.00  0.00           H
ATOM   2124  HA  VAL A 300      18.190  41.673   0.265  1.00  0.00           H
ATOM   2125  HB  VAL A 300      17.920  41.401   2.622  1.00  0.00           H
ATOM   2126  1HG1 VAL A 300      20.235  40.500   2.937  1.00  0.00           H
ATOM   2127  2HG1 VAL A 300      19.677  40.175   1.279  1.00  0.00           H
ATOM   2128  3HG1 VAL A 300      20.814  41.508   1.590  1.00  0.00           H
ATOM   2129  1HG2 VAL A 300      19.408  42.416   4.197  1.00  0.00           H
ATOM   2130  2HG2 VAL A 300      19.972  43.548   2.946  1.00  0.00           H
ATOM   2131  3HG2 VAL A 300      18.272  43.576   3.470  1.00  0.00           H
ATOM   2132  N   TYR A 301      15.978  42.975   0.777  1.00  0.00           N
ATOM   2133  CA  TYR A 301      14.814  43.778   0.444  1.00  0.00           C
ATOM   2134  C   TYR A 301      13.573  43.079   0.998  1.00  0.00           C
ATOM   2135  O   TYR A 301      13.425  41.864   0.846  1.00  0.00           O
ATOM   2136  CB  TYR A 301      14.739  43.992  -1.081  1.00  0.00           C
ATOM   2137  CG  TYR A 301      15.182  42.820  -1.945  1.00  0.00           C
ATOM   2138  CD1 TYR A 301      14.244  41.944  -2.521  1.00  0.00           C
ATOM   2139  CD2 TYR A 301      16.550  42.590  -2.186  1.00  0.00           C
ATOM   2140  CE1 TYR A 301      14.667  40.859  -3.310  1.00  0.00           C
ATOM   2141  CE2 TYR A 301      16.978  41.484  -2.936  1.00  0.00           C
ATOM   2142  CZ  TYR A 301      16.038  40.606  -3.502  1.00  0.00           C
ATOM   2143  OH  TYR A 301      16.443  39.522  -4.226  1.00  0.00           O
ATOM   2144  H   TYR A 301      15.846  41.977   0.850  1.00  0.00           H
ATOM   2145  HA  TYR A 301      14.942  44.786   0.837  1.00  0.00           H
ATOM   2146  1HB TYR A 301      13.710  44.206  -1.368  1.00  0.00           H
ATOM   2147  2HB TYR A 301      15.377  44.830  -1.362  1.00  0.00           H
ATOM   2148  HD1 TYR A 301      13.188  42.100  -2.359  1.00  0.00           H
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ATOM   2149  HD2 TYR A 301      17.290  43.271  -1.790  1.00  0.00           H
ATOM   2150  HE1 TYR A 301      13.937  40.212  -3.774  1.00  0.00           H
ATOM   2151  HE2 TYR A 301      18.034  41.305  -3.081  1.00  0.00           H
ATOM   2152  HH  TYR A 301      17.402  39.499  -4.259  1.00  0.00           H
ATOM   2153  N   GLY A 302      12.722  43.836   1.690  1.00  0.00           N
ATOM   2154  CA  GLY A 302      11.485  43.345   2.273  1.00  0.00           C
ATOM   2155  C   GLY A 302      10.548  42.731   1.230  1.00  0.00           C
ATOM   2156  O   GLY A 302      10.742  42.893   0.026  1.00  0.00           O
ATOM   2157  H   GLY A 302      12.921  44.815   1.836  1.00  0.00           H
ATOM   2158  1HA GLY A 302      11.711  42.578   3.014  1.00  0.00           H
ATOM   2159  2HA GLY A 302      10.957  44.170   2.754  1.00  0.00           H
ATOM   2160  N   GLY A 303       9.537  41.994   1.689  1.00  0.00           N
ATOM   2161  CA  GLY A 303       8.539  41.394   0.817  1.00  0.00           C
ATOM   2162  C   GLY A 303       9.040  40.050   0.292  1.00  0.00           C
ATOM   2163  O   GLY A 303       8.352  39.039   0.387  1.00  0.00           O
ATOM   2164  H   GLY A 303       9.441  41.831  2.682  1.00  0.00           H
ATOM   2165  1HA GLY A 303       7.615  41.238   1.374  1.00  0.00           H
ATOM   2166  2HA GLY A 303       8.347  42.057  -0.026  1.00  0.00           H
ATOM   2167  N   ALA A 304      10.250  40.038  -0.266  1.00  0.00           N
ATOM   2168  CA  ALA A 304      10.794  38.859  -0.914  1.00  0.00           C
ATOM   2169  C   ALA A 304      11.077  37.750   0.101  1.00  0.00           C
ATOM   2170  O   ALA A 304      11.351  38.028   1.273  1.00  0.00           O
ATOM   2171  CB  ALA A 304      12.075  39.240  -1.656  1.00  0.00           C
ATOM   2172  H   ALA A 304      10.823  40.869  -0.247  1.00  0.00           H
ATOM   2173  HA  ALA A 304      10.095  38.506  -1.672  1.00  0.00           H
ATOM   2174  1HB ALA A 304      12.488  38.357  -2.145  1.00  0.00           H
ATOM   2175  2HB ALA A 304      11.851  39.998  -2.405  1.00  0.00           H
ATOM   2176  3HB ALA A 304      12.802  39.635  -0.946  1.00  0.00           H
ATOM   2177  N   ASP A 305      11.078  36.502  -0.382  1.00  0.00           N
ATOM   2178  CA  ASP A 305      11.501  35.325   0.367  1.00  0.00           C
ATOM   2179  C   ASP A 305      12.806  35.634   1.105  1.00  0.00           C
ATOM   2180  O   ASP A 305      13.834  35.883   0.472  1.00  0.00           O
ATOM   2181  CB  ASP A 305      11.704  34.142  -0.597  1.00  0.00           C
ATOM   2182  CG  ASP A 305      12.380  32.954   0.073  1.00  0.00           C
ATOM   2183  OD1 ASP A 305      12.213  32.800   1.298  1.00  0.00           O
ATOM   2184  OD2 ASP A 305      13.125  32.230  -0.628  1.00  0.00          Ol-
ATOM   2185  H   ASP A 305      10.771  36.326  -1.327  1.00  0.00           H
ATOM   2186  HA  ASP A 305      10.723  35.046   1.077  1.00  0.00           H
ATOM   2187  1HB ASP A 305      10.737  33.810  -0.974  1.00  0.00           H
ATOM   2188  2HB ASP A 305      12.331  34.457  -1.432  1.00  0.00           H
ATOM   2189  N   ILE A 306      12.773  35.601   2.438  1.00  0.00           N
ATOM   2190  CA  ILE A 306      13.958  35.726   3.270  1.00  0.00           C
ATOM   2191  C   ILE A 306      15.004  34.708   2.805  1.00  0.00           C
ATOM   2192  O   ILE A 306      16.204  34.982   2.787  1.00  0.00           O
ATOM   2193  CB  ILE A 306      13.570  35.547   4.754  1.00  0.00           C
ATOM   2194  CGI ILE A 306      14.736  35.965   5.665  1.00  0.00           C
ATOM   2195  CG2 ILE A 306      13.081  34.123   5.069  1.00  0.00           C
ATOM   2196  CD1 ILE A 306      14.466  35.723   7.151  1.00  0.00           C
ATOM   2197  H   ILE A 306      11.893  35.484   2.918  1.00  0.00           H
ATOM   2198  HA  ILE A 306      14.323  36.752   3.231  1.00  0.00           H
ATOM   2199  HB  ILE A 306      12.644  36.086   4.956  1.00  0.00           H
ATOM   2200  1HG1 ILE A 306      15.627  35.398   5.398  1.00  0.00           H
ATOM   2201  2HG1 ILE A 306      14.932  37.030   5.538  1.00  0.00           H
ATOM   2202  1HG2 ILE A 306      12.821  34.053   6.125  1.00  0.00           H
ATOM   2203  2HG2 ILE A 306      12.202  33.898   4.464  1.00  0.00           H
ATOM   2204  3HG2 ILE A 306      13.871  33.408   4.841  1.00  0.00           H
ATOM   2205  1HD1 ILE A 306      15.330  36.041   7.735  1.00  0.00           H
ATOM   2206  2HD1 ILE A 306      13.590  36.294   7.460  1.00  0.00           H
ATOM   2207  3HD1 ILE A 306      14.285  34.662   7.320  1.00  0.00           H
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ATOM   2208  N   GLY A 307      14.533  33.529   2.414  1.00  0.00           N
ATOM   2209  CA  GLY A 307      15.319  32.462   1.860  1.00  0.00           C
ATOM   2210  C   GLY A 307      16.163  32.949   0.686  1.00  0.00           C
ATOM   2211  O   GLY A 307      17.314  32.550   0.568  1.00  0.00           O
ATOM   2212  H   GLY A 307      13.547  33.326   2.495  1.00  0.00           H
ATOM   2213  1HA GLY A 307      15.986  32.066   2.626  1.00  0.00           H
ATOM   2214  2HA GLY A 307      14.659  31.669   1.509  1.00  0.00           H
ATOM   2215  N   GLN A 308      15.624  33.783  -0.204  1.00  0.00           N
ATOM   2216  CA  GLN A 308      16.333  34.243  -1.391  1.00  0.00           C
ATOM   2217  C   GLN A 308      17.581  35.024  -0.997  1.00  0.00           C
ATOM   2218  O   GLN A 308      18.546  35.083  -1.756  1.00  0.00           O
ATOM   2219  CB  GLN A 308      15.381  35.073  -2.272  1.00  0.00           C
ATOM   2220  CG  GLN A 308      15.941  35.518  -3.633  1.00  0.00           C
ATOM   2221  CD  GLN A 308      16.122  34.381  -4.635  1.00  0.00           C
ATOM   2222  NE2 GLN A 308      16.133  34.700  -5.921  1.00  0.00           N
ATOM   2223  OE1 GLN A 308      16.234  33.211  -4.272  1.00  0.00           O
ATOM   2224  H   GLN A 308      14.683  34.125  -0.070  1.00  0.00           H
ATOM   2225  HA  GLN A 308      16.565  33.390  -2.030  1.00  0.00           H
ATOM   2226  1HB GLN A 308      14.485  34.492  -2.488  1.00  0.00           H
ATOM   2227  2HB GLN A 308      15.103  35.986  -1.746  1.00  0.00           H
ATOM   2228  1HG GLN A 308      15.262  36.240  -4.087  1.00  0.00           H
ATOM   2229  2HG GLN A 308      16.919  35.979  -3.492  1.00  0.00           H
ATOM   2230  1HE2 GLN A 308      16.250  33.979  -6.619  1.00  0.00           H
ATOM   2231  2HE2 GLN A 308      16.025  35.663  -6.203  1.00  0.00           H
ATOM   2232  N   GLN A 309      17.545  35.625   0.185  1.00  0.00           N
ATOM   2233  CA  GLN A 309      18.573  36.518   0.666  1.00  0.00           C
ATOM   2234  C   GLN A 309      19.501  35.729   1.595  1.00  0.00           C
ATOM   2235  O   GLN A 309      20.710  35.945   1.589  1.00  0.00           O
ATOM   2236  CB  GLN A 309      17.870  37.714   1.312  1.00  0.00           C
ATOM   2237  CG  GLN A 309      17.142  38.529   0.224  1.00  0.00           C
ATOM   2238  CD  GLN A 309      16.001  39.382   0.761  1.00  0.00           C
ATOM   2239  NE2 GLN A 309      15.404  40.198  -0.091  1.00  0.00           N
ATOM   2240  OE1 GLN A 309      15.640  39.322   1.929  1.00  0.00           O
ATOM   2241  H   GLN A 309      16.766  35.469   0.808  1.00  0.00           H
ATOM   2242  HA  GLN A 309      19.082  36.977  -0.182  1.00  0.00           H
ATOM   2243  1HB GLN A 309      17.146  37.357   2.045  1.00  0.00           H
ATOM   2244  2HB GLN A 309      18.607  38.345   1.807  1.00  0.00           H
ATOM   2245  1HG GLN A 309      17.849  39.201  -0.261  1.00  0.00           H
ATOM   2246  2HG GLN A 309      16.719  37.851  -0.517  1.00  0.00           H
ATOM   2247  1HE2 GLN A 309      14.642  40.783   0.221  1.00  0.00           H
ATOM   2248  2HE2 GLN A 309      15.709  40.236  -1.053  1.00  0.00           H
ATOM   2249  N   ILE A 310      18.967  34.758   2.342  1.00  0.00           N
ATOM   2250  CA  ILE A 310      19.774  33.761   3.035  1.00  0.00           C
ATOM   2251  C   ILE A 310      20.632  33.034   1.995  1.00  0.00           C
ATOM   2252  O   ILE A 310      21.827  32.826   2.204  1.00  0.00           O
ATOM   2253  CB  ILE A 310      18.872  32.792   3.830  1.00  0.00           C
ATOM   2254  CGI ILE A 310      18.234  33.536   5.017  1.00  0.00           C
ATOM   2255  CG2 ILE A 310      19.644  31.565   4.344  1.00  0.00           C
ATOM   2256  CD1 ILE A 310      17.119  32.750   5.714  1.00  0.00           C
ATOM   2257  H   ILE A 310      17.964  34.694   2.445  1.00  0.00           H
ATOM   2258  HA  ILE A 310      20.369  34.247   3.808  1.00  0.00           H
ATOM   2259  HB  ILE A 310      18.109  32.380   3.169  1.00  0.00           H
ATOM   2260  1HG1 ILE A 310      18.997  33.748   5.766  1.00  0.00           H
ATOM   2261  2HG1 ILE A 310      17.799  34.473   4.668  1.00  0.00           H
ATOM   2262  1HG2 ILE A 310      18.966  30.914   4.897  1.00  0.00           H
ATOM   2263  2HG2 ILE A 310      20.064  31.019   3.500  1.00  0.00           H
ATOM   2264  3HG2 ILE A 310      20.450  31.891   5.002  1.00  0.00           H
ATOM   2265  1HD1 ILE A 310      16.719  33.340   6.539  1.00  0.00           H
ATOM   2266  2HD1 ILE A 310      16.323  32.538   5.001  1.00  0.00           H
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ATOM   2267 3HD1 ILE A 310      17.521  31.813   6.099  1.00  0.00          H
ATOM   2268  N   ARG A 311      20.030  32.681   0.857  1.00  0.00          N
ATOM   2269  CA  ARG A 311      20.674  31.976  -0.241  1.00  0.00          C
ATOM   2270  C   ARG A 311      21.741  32.839  -0.940  1.00  0.00          C
ATOM   2271  O   ARG A 311      22.281  32.404  -1.963  1.00  0.00          O
ATOM   2272  CB  ARG A 311      19.617  31.454  -1.245  1.00  0.00          C
ATOM   2273  CG  ARG A 311      18.820  30.240  -0.725  1.00  0.00          C
ATOM   2274  CD  ARG A 311      17.788  29.682  -1.730  1.00  0.00          C
ATOM   2275  NE  ARG A 311      16.835  30.684  -2.259  1.00  0.00          N
ATOM   2276  CZ  ARG A 311      15.567  30.904  -1.864  1.00  0.00          C
ATOM   2277  NH1 ARG A 311      15.074  30.373  -0.750  1.00  0.00          N1+
ATOM   2278  NH2 ARG A 311      14.778  31.691  -2.584  1.00  0.00          N
ATOM   2279  H   ARG A 311      19.055  32.902   0.711  1.00  0.00          H
ATOM   2280  HA  ARG A 311      21.084  31.033   0.123  1.00  0.00          H
ATOM   2281 1HB  ARG A 311      18.900  32.246  -1.463  1.00  0.00          H
ATOM   2282 2HB  ARG A 311      20.111  31.149  -2.168  1.00  0.00          H
ATOM   2283 1HG  ARG A 311      19.507  29.428  -0.488  1.00  0.00          H
ATOM   2284 2HG  ARG A 311      18.271  30.523   0.173  1.00  0.00          H
ATOM   2285 1HD  ARG A 311      18.309  29.258  -2.589  1.00  0.00          H
ATOM   2286 2HD  ARG A 311      17.193  28.906  -1.248  1.00  0.00          H
ATOM   2287  HE  ARG A 311      17.237  31.239  -3.001  1.00  0.00          H
ATOM   2288 1HH1 ARG A 311      14.118  30.558  -0.482  1.00  0.00          H
ATOM   2289 2HH1 ARG A 311      15.656  29.783  -0.172  1.00  0.00          H
ATOM   2290 1HH2 ARG A 311      13.827  31.857  -2.289  1.00  0.00          H
ATOM   2291 2HH2 ARG A 311      15.129  32.123  -3.426  1.00  0.00          H
ATOM   2292  N   ASP A 312      22.066  34.029  -0.416  1.00  0.00          N
ATOM   2293  CA  ASP A 312      23.196  34.840  -0.850  1.00  0.00          C
ATOM   2294  C   ASP A 312      24.067  35.280   0.327  1.00  0.00          C
ATOM   2295  O   ASP A 312      25.284  35.096   0.293  1.00  0.00          O
ATOM   2296  CB  ASP A 312      22.750  36.035  -1.693  1.00  0.00          C
ATOM   2297  CG  ASP A 312      23.957  36.804  -2.202  1.00  0.00          C
ATOM   2298  OD1 ASP A 312      24.970  36.166  -2.562  1.00  0.00          O
ATOM   2299  OD2 ASP A 312      23.912  38.045  -2.233  1.00  0.00          Ol-
ATOM   2300  H   ASP A 312      21.512  34.420   0.332  1.00  0.00          H
ATOM   2301  HA  ASP A 312      23.758  34.302  -1.614  1.00  0.00          H
ATOM   2302 1HB  ASP A 312      22.169  35.683  -2.545  1.00  0.00          H
ATOM   2303 2HB  ASP A 312      22.137  36.700  -1.086  1.00  0.00          H
ATOM   2304  N   LEU A 313      23.465  35.852   1.370  1.00  0.00          N
ATOM   2305  CA  LEU A 313      24.189  36.307   2.550  1.00  0.00          C
ATOM   2306  C   LEU A 313      25.117  35.215   3.072  1.00  0.00          C
ATOM   2307  O   LEU A 313      26.282  35.474   3.362  1.00  0.00          O
ATOM   2308  CB  LEU A 313      23.227  36.694   3.681  1.00  0.00          C
ATOM   2309  CG  LEU A 313      22.531  38.052   3.513  1.00  0.00          C
ATOM   2310  CD1 LEU A 313      21.519  38.189   4.656  1.00  0.00          C
ATOM   2311  CD2 LEU A 313      23.529  39.215   3.586  1.00  0.00          C
ATOM   2312  H   LEU A 313      22.463  35.986   1.364  1.00  0.00          H
ATOM   2313  HA  LEU A 313      24.783  37.185   2.296  1.00  0.00          H
ATOM   2314 1HB  LEU A 313      22.435  35.949   3.756  1.00  0.00          H
ATOM   2315 2HB  LEU A 313      23.772  36.741   4.623  1.00  0.00          H
ATOM   2316  HG  LEU A 313      22.017  38.081   2.552  1.00  0.00          H
ATOM   2317 1HD1 LEU A 313      21.002  39.145   4.572  1.00  0.00          H
ATOM   2318 2HD1 LEU A 313      20.793  37.377   4.599  1.00  0.00          H
ATOM   2319 3HD1 LEU A 313      22.041  38.142   5.612  1.00  0.00          H
ATOM   2320 1HD2 LEU A 313      22.997  40.158   3.463  1.00  0.00          H
ATOM   2321 2HD2 LEU A 313      24.030  39.204   4.554  1.00  0.00          H
ATOM   2322 3HD2 LEU A 313      24.269  39.109   2.793  1.00  0.00          H
ATOM   2323  N   GLU A 314      24.596  33.996   3.216  1.00  0.00          N
ATOM   2324  CA  GLU A 314      25.322  32.929   3.875  1.00  0.00          C
ATOM   2325  C   GLU A 314      26.442  32.358   2.998  1.00  0.00          C
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ATOM   2326  O   GLU A 314      27.173  31.472   3.454  1.00  0.00           O
ATOM   2327  CB  GLU A 314      24.326  31.861   4.344  1.00  0.00           C
ATOM   2328  CG  GLU A 314      23.537  32.367   5.564  1.00  0.00           C
ATOM   2329  CD  GLU A 314      23.421  31.295   6.630  1.00  0.00           C
ATOM   2330  OE1 GLU A 314      24.479  30.922   7.176  1.00  0.00           O
ATOM   2331  OE2 GLU A 314      22.282  30.869   6.909  1.00  0.00           Ol-
ATOM   2332  H   GLU A 314      23.672  33.797   2.861  1.00  0.00           H
ATOM   2333  HA  GLU A 314      25.682  33.278   4.843  1.00  0.00           H
ATOM   2334  1HB GLU A 314      23.628  31.635   3.537  1.00  0.00           H
ATOM   2335  2HB GLU A 314      24.866  30.955   4.620  1.00  0.00           H
ATOM   2336  1HG GLU A 314      24.047  33.229   5.995  1.00  0.00           H
ATOM   2337  2HG GLU A 314      22.533  32.658   5.254  1.00  0.00           H
ATOM   2338  N   ARG A 315      26.594  32.852   1.766  1.00  0.00           N
ATOM   2339  CA  ARG A 315      27.792  32.608   0.980  1.00  0.00           C
ATOM   2340  C   ARG A 315      28.940  33.437   1.566  1.00  0.00           C
ATOM   2341  O   ARG A 315      30.093  33.020   1.525  1.00  0.00           O
ATOM   2342  CB  ARG A 315      27.587  33.030  -0.485  1.00  0.00           C
ATOM   2343  CG  ARG A 315      26.358  32.416  -1.172  1.00  0.00           C
ATOM   2344  CD  ARG A 315      26.188  33.043  -2.567  1.00  0.00           C
ATOM   2345  NE  ARG A 315      24.855  32.769  -3.133  1.00  0.00           N
ATOM   2346  CZ  ARG A 315      24.233  33.493  -4.079  1.00  0.00           C
ATOM   2347  NH1 ARG A 315      24.816  34.563  -4.614  1.00  0.00           N1+
ATOM   2348  NH2 ARG A 315      23.009  33.136  -4.457  1.00  0.00           N
ATOM   2349  H   ARG A 315      25.864  33.414   1.353  1.00  0.00           H
ATOM   2350  HA  ARG A 315      28.052  31.550   1.032  1.00  0.00           H
ATOM   2351  1HB ARG A 315      27.466  34.112  -0.538  1.00  0.00           H
ATOM   2352  2HB ARG A 315      28.455  32.733  -1.074  1.00  0.00           H
ATOM   2353  1HG ARG A 315      26.496  31.339  -1.271  1.00  0.00           H
ATOM   2354  2HG ARG A 315      25.469  32.615  -0.573  1.00  0.00           H
ATOM   2355  1HD ARG A 315      26.315  34.124  -2.498  1.00  0.00           H
ATOM   2356  2HD ARG A 315      26.937  32.632  -3.244  1.00  0.00           H
ATOM   2357  HE  ARG A 315      24.404  31.953  -2.745  1.00  0.00           H
ATOM   2358  1HH1 ARG A 315      24.336  35.097  -5.324  1.00  0.00           H
ATOM   2359  2HH1 ARG A 315      25.738  34.841  -4.309  1.00  0.00           H
ATOM   2360  1HH2 ARG A 315      22.524  33.667  -5.167  1.00  0.00           H
ATOM   2361  2HH2 ARG A 315      22.563  32.334  -4.035  1.00  0.00           H
ATOM   2362  N   GLY A 316      28.619  34.645   2.025  1.00  0.00           N
ATOM   2363  CA  GLY A 316      29.575  35.645   2.465  1.00  0.00           C
ATOM   2364  C   GLY A 316      28.996  37.028   2.158  1.00  0.00           C
ATOM   2365  O   GLY A 316      28.255  37.173   1.183  1.00  0.00           O
ATOM   2366  H   GLY A 316      27.650  34.922   2.086  1.00  0.00           H
ATOM   2367  1HA GLY A 316      29.745  35.539   3.536  1.00  0.00           H
ATOM   2368  2HA GLY A 316      30.517  35.507   1.933  1.00  0.00           H
ATOM   2369  N   CYS A 317      29.325  38.057   2.941  1.00  0.00           N
ATOM   2370  CA  CYS A 317      28.883  39.428   2.711  1.00  0.00           C
ATOM   2371  C   CYS A 317      29.800  40.358   3.506  1.00  0.00           C
ATOM   2372  O   CYS A 317      29.919  40.199   4.718  1.00  0.00           O
ATOM   2373  CB  CYS A 317      27.417  39.563   3.144  1.00  0.00           C
ATOM   2374  SG  CYS A 317      26.883  41.294   3.166  1.00  0.00           S
ATOM   2375  H   CYS A 317      29.914  37.909   3.748  1.00  0.00           H
ATOM   2376  HA  CYS A 317      28.915  39.647   1.644  1.00  0.00           H
ATOM   2377  1HB CYS A 317      26.780  39.016   2.449  1.00  0.00           H
ATOM   2378  2HB CYS A 317      27.295  39.154   4.147  1.00  0.00           H
ATOM   2379  HG  CYS A 317      25.830  41.349   3.481  1.00  0.00           H
ATOM   2380  N   HIS A 318      30.474  41.300   2.834  1.00  0.00           N
ATOM   2381  CA  HIS A 318      31.444  42.193   3.470  1.00  0.00           C
ATOM   2382  C   HIS A 318      30.885  43.617   3.531  1.00  0.00           C
ATOM   2383  O   HIS A 318      31.498  44.502   4.124  1.00  0.00           O
ATOM   2384  CB  HIS A 318      32.753  42.250   2.666  1.00  0.00           C
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ATOM   2385  CG  HIS A 318      33.410  40.942   2.291  1.00  0.00           C
ATOM   2386  CD2 HIS A 318      33.040  39.623   2.415  1.00  0.00           C
ATOM   2387  ND1 HIS A 318      34.653  40.909   1.664  1.00  0.00           N
ATOM   2388  CE1 HIS A 318      34.952  39.628   1.393  1.00  0.00           C
ATOM   2389  NE2 HIS A 318      33.990  38.814   1.816  1.00  0.00           N
ATOM   2390  H   HIS A 318     30.323  41.419   1.843  1.00  0.00           H
ATOM   2391  HA  HIS A 318      31.632  41.859   4.490  1.00  0.00           H
ATOM   2392  1HB HIS A 318      32.577  42.761   1.719  1.00  0.00           H
ATOM   2393  2HB HIS A 318      33.507  42.793   3.236  1.00  0.00           H
ATOM   2394  HD2 HIS A 318      32.124  39.365   2.925  1.00  0.00           H
ATOM   2395  HD1 HIS A 318      35.156  41.769   1.494  1.00  0.00           H
ATOM   2396  HE1 HIS A 318      35.877  39.384   0.892  1.00  0.00           H
ATOM   2397  N   LEU A 319      29.761  43.855   2.861  1.00  0.00           N
ATOM   2398  CA  LEU A 319      29.164  45.163   2.645  1.00  0.00           C
ATOM   2399  C   LEU A 319      27.727  44.879   2.219  1.00  0.00           C
ATOM   2400  O   LEU A 319      27.492  43.890   1.521  1.00  0.00           O
ATOM   2401  CB  LEU A 319      29.957  45.938   1.577  1.00  0.00           C
ATOM   2402  CG  LEU A 319      29.459  47.383   1.376  1.00  0.00           C
ATOM   2403  CD1 LEU A 319      30.645  48.298   1.041  1.00  0.00           C
ATOM   2404  CD2 LEU A 319      28.433  47.494   0.240  1.00  0.00           C
ATOM   2405  H   LEU A 319      29.247  43.090   2.449  1.00  0.00           H
ATOM   2406  HA  LEU A 319      29.227  45.748   3.562  1.00  0.00           H
ATOM   2407  1HB LEU A 319      31.005  45.990   1.870  1.00  0.00           H
ATOM   2408  2HB LEU A 319      29.872  45.426   0.619  1.00  0.00           H
ATOM   2409  HG  LEU A 319      28.976  47.732   2.289  1.00  0.00           H
ATOM   2410  1HD1 LEU A 319     30.288  49.318   0.899  1.00  0.00           H
ATOM   2411  2HD1 LEU A 319     31.365  48.275   1.858  1.00  0.00           H
ATOM   2412  3HD1 LEU A 319     31.124  47.951   0.125  1.00  0.00           H
ATOM   2413  1HD2 LEU A 319     28.114  48.532   0.138  1.00  0.00           H
ATOM   2414  2HD2 LEU A 319     28.887  47.161  -0.694  1.00  0.00           H
ATOM   2415  3HD2 LEU A 319     27.569  46.870   0.467  1.00  0.00           H
ATOM   2416  N   LEU A 320      26.768  45.678   2.676  1.00  0.00           N
ATOM   2417  CA  LEU A 320      25.365  45.306   2.623  1.00  0.00           C
ATOM   2418  C   LEU A 320      24.502  46.547   2.448  1.00  0.00           C
ATOM   2419  O   LEU A 320      24.774  47.571   3.073  1.00  0.00           O
ATOM   2420  CB  LEU A 320      25.026  44.603   3.940  1.00  0.00           C
ATOM   2421  CG  LEU A 320      23.575  44.115   4.057  1.00  0.00           C
ATOM   2422  CD1 LEU A 320      23.172  43.159   2.930  1.00  0.00           C
ATOM   2423  CD2 LEU A 320      23.466  43.354   5.376  1.00  0.00           C
ATOM   2424  H   LEU A 320      27.005  46.575   3.075  1.00  0.00           H
ATOM   2425  HA  LEU A 320      25.199  44.629   1.785  1.00  0.00           H
ATOM   2426  1HB LEU A 320      25.662  43.725   4.059  1.00  0.00           H
ATOM   2427  2HB LEU A 320      25.194  45.287   4.772  1.00  0.00           H
ATOM   2428  HG  LEU A 320      22.898  44.967   3.994  1.00  0.00           H
ATOM   2429  1HD1 LEU A 320     22.136  42.850   3.069  1.00  0.00           H
ATOM   2430  2HD1 LEU A 320     23.275  43.664   1.970  1.00  0.00           H
ATOM   2431  3HD1 LEU A 320     23.818  42.281   2.949  1.00  0.00           H
ATOM   2432  1HD2 LEU A 320     22.447  42.987   5.501  1.00  0.00           H
ATOM   2433  2HD2 LEU A 320     24.157  42.511   5.367  1.00  0.00           H
ATOM   2434  3HD2 LEU A 320     23.716  44.020   6.202  1.00  0.00           H
ATOM   2435  N   VAL A 321      23.452  46.431   1.637  1.00  0.00           N
ATOM   2436  CA  VAL A 321      22.434  47.453   1.469  1.00  0.00           C
ATOM   2437  C   VAL A 321      21.093  46.812   1.845  1.00  0.00           C
ATOM   2438  O   VAL A 321      20.824  45.687   1.413  1.00  0.00           O
ATOM   2439  CB  VAL A 321      22.436  47.962   0.018  1.00  0.00           C
ATOM   2440  CGI VAL A 321      21.572  49.223  -0.067  1.00  0.00           C
ATOM   2441  CG2 VAL A 321      23.849  48.280  -0.496  1.00  0.00           C
ATOM   2442  H   VAL A 321      23.327  45.591   1.090  1.00  0.00           H
ATOM   2443  HA  VAL A 321      22.669  48.308   2.103  1.00  0.00           H
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ATOM   2444  HB  VAL A 321      22.052  47.183  -0.641  1.00  0.00           H
ATOM   2445 1HG1 VAL A 321      21.567  49.592  -1.093  1.00  0.00           H
ATOM   2446 2HG1 VAL A 321      20.553  48.987   0.238  1.00  0.00           H
ATOM   2447 3HG1 VAL A 321      21.981  49.989   0.591  1.00  0.00           H
ATOM   2448 1HG2 VAL A 321      23.790  48.635  -1.525  1.00  0.00           H
ATOM   2449 2HG2 VAL A 321      24.298  49.052   0.129  1.00  0.00           H
ATOM   2450 3HG2 VAL A 321      24.461  47.379  -0.457  1.00  0.00           H
ATOM   2451  N   ALA A 322      20.264  47.466   2.662  1.00  0.00           N
ATOM   2452  CA  ALA A 322      19.098  46.813   3.244  1.00  0.00           C
ATOM   2453  C   ALA A 322      17.926  47.764   3.486  1.00  0.00           C
ATOM   2454  O   ALA A 322      18.103  48.840   4.048  1.00  0.00           O
ATOM   2455  CB  ALA A 322      19.506  46.165   4.567  1.00  0.00           C
ATOM   2456  H   ALA A 322      20.439  48.435   2.889  1.00  0.00           H
ATOM   2457  HA  ALA A 322      18.769  46.005   2.590  1.00  0.00           H
ATOM   2458 1HB  ALA A 322      18.642  45.673   5.012  1.00  0.00           H
ATOM   2459 2HB  ALA A 322      20.289  45.429   4.385  1.00  0.00           H
ATOM   2460 3HB  ALA A 322      19.878  46.931   5.247  1.00  0.00           H
ATOM   2461  N   THR A 323      16.710  47.332   3.147  1.00  0.00           N
ATOM   2462  CA  THR A 323      15.513  47.989   3.643  1.00  0.00           C
ATOM   2463  C   THR A 323      15.367  47.574   5.120  1.00  0.00           C
ATOM   2464  O   THR A 323      15.319  46.365   5.365  1.00  0.00           O
ATOM   2465  CB  THR A 323      14.306  47.518   2.811  1.00  0.00           C
ATOM   2466  CG2 THR A 323      14.396  48.006   1.361  1.00  0.00           C
ATOM   2467  OG1 THR A 323      14.239  46.100   2.807  1.00  0.00           O
ATOM   2468  H   THR A 323      16.610  46.534   2.535  1.00  0.00           H
ATOM   2469  HA  THR A 323      15.626  49.069   3.552  1.00  0.00           H
ATOM   2470  HB  THR A 323      13.387  47.899   3.256  1.00  0.00           H
ATOM   2471 1HG2 THR A 323      13.528  47.654   0.804  1.00  0.00           H
ATOM   2472 2HG2 THR A 323      14.421  49.096   1.345  1.00  0.00           H
ATOM   2473 3HG2 THR A 323      15.304  47.616   0.901  1.00  0.00           H
ATOM   2474  HG1 THR A 323      13.484  45.816   2.286  1.00  0.00           H
ATOM   2475  N   PRO A 324      15.269  48.496   6.095  1.00  0.00           N
ATOM   2476  CA  PRO A 324      15.544  48.216   7.502  1.00  0.00           C
ATOM   2477  C   PRO A 324      14.872  46.960   8.068  1.00  0.00           C
ATOM   2478  O   PRO A 324      15.510  46.140   8.729  1.00  0.00           O
ATOM   2479  CB  PRO A 324      15.093  49.474   8.242  1.00  0.00           C
ATOM   2480  CG  PRO A 324      15.494  50.578   7.268  1.00  0.00           C
ATOM   2481  CD  PRO A 324      15.309  49.942   5.885  1.00  0.00           C
ATOM   2482  HA  PRO A 324      16.620  48.132   7.653  1.00  0.00           H
ATOM   2483 1HB  PRO A 324      14.017  49.428   8.415  1.00  0.00           H
ATOM   2484 2HB  PRO A 324      15.611  49.540   9.198  1.00  0.00           H
ATOM   2485 1HG  PRO A 324      14.847  51.443   7.411  1.00  0.00           H
ATOM   2486 2HG  PRO A 324      16.530  50.866   7.451  1.00  0.00           H
ATOM   2487 1HD  PRO A 324      16.141  50.191   5.227  1.00  0.00           H
ATOM   2488 2HD  PRO A 324      14.375  50.269   5.429  1.00  0.00           H
ATOM   2489  N   GLY A 325      13.578  46.794   7.797  1.00  0.00           N
ATOM   2490  CA  GLY A 325      12.819  45.667   8.312  1.00  0.00           C
ATOM   2491  C   GLY A 325      13.486  44.338   7.947  1.00  0.00           C
ATOM   2492  O   GLY A 325      13.493  43.402   8.742  1.00  0.00           O
ATOM   2493  H   GLY A 325      13.094  47.463   7.216  1.00  0.00           H
ATOM   2494 1HA  GLY A 325      12.756  45.737   9.398  1.00  0.00           H
ATOM   2495 2HA  GLY A 325      11.815  45.680   7.888  1.00  0.00           H
ATOM   2496  N   ARG A 326      14.086  44.261   6.756  1.00  0.00           N
ATOM   2497  CA  ARG A 326      14.723  43.054   6.254  1.00  0.00           C
ATOM   2498  C   ARG A 326      16.220  43.070   6.585  1.00  0.00           C
ATOM   2499  O   ARG A 326      17.026  42.392   5.949  1.00  0.00           O
ATOM   2500  CB  ARG A 326      14.394  42.886   4.763  1.00  0.00           C
ATOM   2501  CG  ARG A 326      15.010  41.669   4.053  1.00  0.00           C
ATOM   2502  CD  ARG A 326      15.002  40.352   4.848  1.00  0.00           C
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ATOM   2503  NE  ARG A 326      13.659  39.845   5.151  1.00  0.00           N
ATOM   2504  CZ  ARG A 326      12.806  39.257   4.310  1.00  0.00           C
ATOM   2505  NH1 ARG A 326      13.064  39.216   3.005  1.00  0.00           N1+
ATOM   2506  NH2 ARG A 326      11.711  38.703   4.818  1.00  0.00           N
ATOM   2507  H   ARG A 326      14.113  45.069   6.151  1.00  0.00           H
ATOM   2508  HA  ARG A 326      14.184  42.179   6.619  1.00  0.00           H
ATOM   2509  1HB ARG A 326      13.316  42.788   4.637  1.00  0.00           H
ATOM   2510  2HB ARG A 326      14.745  43.759   4.212  1.00  0.00           H
ATOM   2511  1HG ARG A 326      14.464  41.470   3.131  1.00  0.00           H
ATOM   2512  2HG ARG A 326      16.055  41.875   3.819  1.00  0.00           H
ATOM   2513  1HD ARG A 326      15.514  39.578   4.275  1.00  0.00           H
ATOM   2514  2HD ARG A 326      15.513  40.497   5.799  1.00  0.00           H
ATOM   2515  HE  ARG A 326      13.401  39.983   6.118  1.00  0.00           H
ATOM   2516  1HH1 ARG A 326     12.414  38.769   2.375  1.00  0.00           H
ATOM   2517  2HH1 ARG A 326     13.911  39.632   2.644  1.00  0.00           H
ATOM   2518  1HH2 ARG A 326     11.045  38.250   4.209  1.00  0.00           H
ATOM   2519  2HH2 ARG A 326     11.544  38.735   5.814  1.00  0.00           H
ATOM   2520  N   LEU A 327      16.597  43.806   7.626  1.00  0.00           N
ATOM   2521  CA  LEU A 327      17.877  43.651  8.284  1.00  0.00           C
ATOM   2522  C   LEU A 327      17.606  43.095   9.677  1.00  0.00           C
ATOM   2523  O   LEU A 327      18.223  42.108  10.074  1.00  0.00           O
ATOM   2524  CB  LEU A 327      18.624  44.985   8.323  1.00  0.00           C
ATOM   2525  CG  LEU A 327      20.113  44.789   8.640  1.00  0.00           C
ATOM   2526  CD1 LEU A 327      20.883  44.162   7.473  1.00  0.00           C
ATOM   2527  CD2 LEU A 327      20.733  46.152   8.924  1.00  0.00           C
ATOM   2528  H   LEU A 327      15.979  44.514   7.994  1.00  0.00           H
ATOM   2529  HA  LEU A 327      18.519  43.005   7.685  1.00  0.00           H
ATOM   2530  1HB LEU A 327      18.541  45.477   7.354  1.00  0.00           H
ATOM   2531  2HB LEU A 327      18.190  45.624   9.092  1.00  0.00           H
ATOM   2532  HG  LEU A 327      20.219  44.118   9.492  1.00  0.00           H
ATOM   2533  1HD1 LEU A 327     21.931  44.045   7.749  1.00  0.00           H
ATOM   2534  2HD1 LEU A 327     20.458  43.186   7.239  1.00  0.00           H
ATOM   2535  3HD1 LEU A 327     20.808  44.809   6.599  1.00  0.00           H
ATOM   2536  1HD2 LEU A 327     21.792  46.031  9.151  1.00  0.00           H
ATOM   2537  2HD2 LEU A 327     20.621  46.792   8.048  1.00  0.00           H
ATOM   2538  3HD2 LEU A 327     20.229  46.611  9.775  1.00  0.00           H
ATOM   2539  N   VAL A 328      16.643  43.679  10.392  1.00  0.00           N
ATOM   2540  CA  VAL A 328      16.180  43.141  11.665  1.00  0.00           C
ATOM   2541  C   VAL A 328      15.821  41.661  11.476  1.00  0.00           C
ATOM   2542  O   VAL A 328      16.260  40.799  12.239  1.00  0.00           O
ATOM   2543  CB  VAL A 328      14.993  43.968  12.194  1.00  0.00           C
ATOM   2544  CGI VAL A 328      14.470  43.384  13.510  1.00  0.00           C
ATOM   2545  CG2 VAL A 328      15.408  45.425  12.438  1.00  0.00           C
ATOM   2546  H   VAL A 328      16.207  44.526  10.055  1.00  0.00           H
ATOM   2547  HA  VAL A 328      16.946  43.294  12.425  1.00  0.00           H
ATOM   2548  HB  VAL A 328      14.191  43.966  11.456  1.00  0.00           H
ATOM   2549  1HG1 VAL A 328     13.632  43.983  13.867  1.00  0.00           H
ATOM   2550  2HG1 VAL A 328     14.139  42.358  13.347  1.00  0.00           H
ATOM   2551  3HG1 VAL A 328     15.266  43.394  14.255  1.00  0.00           H
ATOM   2552  1HG2 VAL A 328     14.553  45.989  12.811  1.00  0.00           H
ATOM   2553  2HG2 VAL A 328     16.212  45.456  13.174  1.00  0.00           H
ATOM   2554  3HG2 VAL A 328     15.754  45.867  11.504  1.00  0.00           H
ATOM   2555  N   ASP A 329      15.077  41.370  10.404  1.00  0.00           N
ATOM   2556  CA  ASP A 329      14.580  40.037  10.081  1.00  0.00           C
ATOM   2557  C   ASP A 329      15.716  39.037   9.810  1.00  0.00           C
ATOM   2558  O   ASP A 329      15.490  37.837   9.679  1.00  0.00           O
ATOM   2559  CB  ASP A 329      13.657  40.159   8.861  1.00  0.00           C
ATOM   2560  CG  ASP A 329      12.850  38.917   8.533  1.00  0.00           C
ATOM   2561  OD1 ASP A 329      12.418  38.234   9.483  1.00  0.00           O
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ATOM 2562 OD2 ASP A 329 12.615 38.707 7.321 1.00 0.00 Ol-
ATOM 2563 H ASP A 329 14.824 42.098 9.75 1 1.00 0.00 H
ATOM 2564 HA ASP A 329 13.953 39.676 10.896 1.00 0.00 H
ATOM 2565 1HB ASP A 329 12.937 40.960 9.027 1.00 0.00 H
ATOM 2566 2HB ASP A 329 14.252 40.384 7.975 1.00 0.00 H
ATOM 2567 N MET A 330 16.950 39.526 9.678 1.00 0.00 N
ATOM 2568 CA MET A 330 18.132 38.723 9.423 1.00 0.00 C
ATOM 2569 C MET A 330 19.016 38.672 10.668 1.00 0.00 C
ATOM 2570 O MET A 330 19.720 37.683 10.881 1.00 0.00 O
ATOM 2571 CB MET A 330 18.898 39.340 8.252 1.00 0.00 C
ATOM 2572 CG MET A 330 18.206 39.083 6.916 1.00 0.00 C
ATOM 2573 SD MET A 330 18.359 37.367 6.355 1.00 0.00 S
ATOM 2574 CE MET A 330 17.908 37.579 4.621 1.00 0.00 C
ATOM 2575 H MET A 330 17.1 10 40.520 9.754 1.00 0.00 H
ATOM 2576 HA MET A 330 17.833 37.715 9.139 1.00 0.00 H
ATOM 2577 1HB MET A 330 18.972 40.41 8 8.393 1.00 0.00 H
ATOM 2578 2HB MET A 330 19.898 38.910 8.204 1.00 0.00 H
ATOM 2579 1HG MET A 330 17. 143 39.307 7.007 1.00 0.00 H
ATOM 2580 2HG MET A 330 18.646 39.721 6. 149 1.00 0.00 H
ATOM 2581 1HE MET A 330 17.949 36.615 4. 114 1.00 0.00 H
ATOM 2582 2HE MET A 330 16.898 37.982 4.555 1.00 0.00 H
ATOM 2583 3HE MET A 330 18.606 38.269 4.146 1.00 0.00 H
ATOM 2584 N MET A 33 1 19.003 39.736 11.466 1.00 0.00 N
ATOM 2585 CA MET A 33 1 19.748 39.833 12.710 1.00 0.00 C
ATOM 2586 C MET A 33 1 19.1 80 38.824 13.700 1.00 0.00 C
ATOM 2587 O MET A 33 1 19.903 37.962 14.201 1.00 0.00 O
ATOM 2588 CB MET A 33 1 19.667 41.263 13.256 1.00 0.00 C
ATOM 2589 CG MET A 33 1 20.5 19 42.21 1 12.406 1.00 0.00 C
ATOM 2590 SD MET A 33 1 20. 126 43.969 12.567 1.00 0.00 S
ATOM 2591 CE MET A 33 1 20.3 10 44. 138 14.354 1.00 0.00 C
ATOM 2592 H MET A 33 1 18.45 1 40.545 11.220 1.00 0.00 H
ATOM 2593 HA MET A 33 1 20.806 39.657 12.5 16 1.00 0.00 H
ATOM 2594 1HB MET A 33 1 18.632 4 1.603 13.234 1.00 0.00 H
ATOM 2595 2HB MET A 33 1 20.034 4 1.282 14.282 1.00 0.00 H
ATOM 2596 1HG MET A 33 1 2 1.568 42.105 12.684 1.00 0.00 H
ATOM 2597 2HG MET A 33 1 20.396 41.964 11.352 1.00 0.00 H
ATOM 2598 1HE MET A 33 1 20.105 45. 169 14.645 1.00 0.00 H
ATOM 2599 2HE MET A 33 1 19.609 43.472 14.857 1.00 0.00 H
ATOM 2600 3HE MET A 33 1 2 1.329 43.877 14.641 1.00 0.00 H
ATOM 2601 N GLU A 332 17.865 38.884 13.920 1.00 0.00 N
ATOM 2602 CA GLU A 332 17.158 38.012 14.846 1.00 0.00 C
ATOM 2603 C GLU A 332 17.308 36.536 14.474 1.00 0.00 C
ATOM 2604 O GLU A 332 16.894 35.655 15.223 1.00 0.00 O
ATOM 2605 CB GLU A 332 15.669 38.344 14.788 1.00 0.00 C
ATOM 2606 CG GLU A 332 15.339 39.729 15.336 1.00 0.00 C
ATOM 2607 CD GLU A 332 13.868 40.056 15.168 1.00 0.00 C
ATOM 2608 OE1 GLU A 332 13.147 39.242 14.544 1.00 0.00 O
ATOM 2609 OE2 GLU A 332 13.508 4 1.130 15.683 1.00 0.00 Ol-
ATOM 2610 H GLU A 332 17.302 39.565 13.43 1 1.00 0.00 H
ATOM 261 1 HA GLU A 332 17.574 38.128 15.847 1.00 0.00 H
ATOM 2612 1HB GLU A 332 15.329 38.3 12 13.752 1.00 0.00 H
ATOM 2613 2HB GLU A 332 15.1 10 37.617 15.376 1.00 0.00 H
ATOM 2614 1HG GLU A 332 15.582 39.767 16.398 1.00 0.00 H
ATOM 2615 2HG GLU A 332 15.922 40.480 14.803 1.00 0.00 H
ATOM 2616 N ARG A 333 17.779 36.259 13.261 1.00 0.00 N
ATOM 2617 CA ARG A 333 17.801 34.93 1 12.684 1.00 0.00 C
ATOM 2618 C ARG A 333 19.250 34.599 12.3 12 1.00 0.00 C
ATOM 2619 O ARG A 333 19.526 33.668 11.554 1.00 0.00 O
ATOM 2620 CB ARG A 333 16.769 34.867 11.540 1.00 0.00 C

ATOM 2621 CG ARG A 333 15.467 35.537 12.028 1.00 0.00 C
ATOM 2622 CD ARG A 333 14.206 35.296 11.188 1.00 0.00 C
ATOM 2623 NE ARG A 333 13.252 36.421 11.270 1.00 0.00 N
ATOM 2624 CZ ARG A 333 12.892 37.163 12.330 1.00 0.00 C
ATOM 2625 NH1 ARG A 333 13.156 36.784 13.575 1.00 0.00 N1+
ATOM 2626 NH2 ARG A 333 12.281 38.321 12.139 1.00 0.00 N
ATOM 2627 H ARG A 333 18.151 36.999 12.682 1.00 0.00 H
ATOM 2628 HA ARG A 333 17.309 34.232 13.361 1.00 0.00 H
ATOM 2629 1HB ARG A 333 17.158 35.394 10.669 1.00 0.00 H
ATOM 2630 2HB ARG A 333 16.579 33.826 11.279 1.00 0.00 H
ATOM 2631 1HG ARG A 333 15.226 35.179 13.029 1.00 0.00 H
ATOM 2632 2HG ARG A 333 15.602 36.619 12.052 1.00 0.00 H
ATOM 2633 1HD ARG A 333 14.485 35.167 10.142 1.00 0.00 H
ATOM 2634 2HD ARG A 333 13.699 34.398 11.541 1.00 0.00 H
ATOM 2635 HE ARG A 333 12.848 36.607 10.363 1.00 0.00 H
ATOM 2636 1HH1 ARG A 333 12.872 37.365 14.351 1.00 0.00 H
ATOM 2637 2HH1 ARG A 333 13.642 35.915 13.747 1.00 0.00 H
ATOM 2638 1HH2 ARG A 333 12.008 38.884 12.932 1.00 0.00 H
ATOM 2639 2HH2 ARG A 333 12.089 38.642 11.201 1.00 0.00 H
ATOM 2640 N GLY A 334 20.185 35.356 12.894 1.00 0.00 N
ATOM 2641 CA GLY A 334 21.579 34.990 13.026 1.00 0.00 C
ATOM 2642 C GLY A 334 22.355 35.110 11.719 1.00 0.00 C
ATOM 2643 O GLY A 334 23.431 34.528 11.602 1.00 0.00 O
ATOM 2644 H GLY A 334 19.938 36.255 13.283 1.00 0.00 H
ATOM 2645 1HA GLY A 334 22.059 35.642 13.756 1.00 0.00 H
ATOM 2646 2HA GLY A 334 21.654 33.955 13.360 1.00 0.00 H
ATOM 2647 N LYS A 335 21.843 35.858 10.742 1.00 0.00 N
ATOM 2648 CA LYS A 335 22.464 35.978 9.430 1.00 0.00 C
ATOM 2649 C LYS A 335 23.287 37.261 9.335 1.00 0.00 C
ATOM 2650 O LYS A 335 24.110 37.399 8.433 1.00 0.00 O
ATOM 2651 CB LYS A 335 21.389 35.962 8.335 1.00 0.00 C
ATOM 2652 CG LYS A 335 20.351 34.843 8.494 1.00 0.00 C
ATOM 2653 CD LYS A 335 21.019 33.466 8.593 1.00 0.00 C
ATOM 2654 CE LYS A 335 19.979 32.341 8.601 1.00 0.00 C
ATOM 2655 NZ LYS A 335 20.613 31.046 8.902 1.00 0.00 N1+
ATOM 2656 H LYS A 335 20.988 36.373 10.895 1.00 0.00 H
ATOM 2657 HA LYS A 335 23.096 35.109 9.246 1.00 0.00 H
ATOM 2658 1HB LYS A 335 20.846 36.907 8.345 1.00 0.00 H
ATOM 2659 2HB LYS A 335 21.862 35.825 7.363 1.00 0.00 H
ATOM 2660 1HG LYS A 335 19.771 35.010 9.401 1.00 0.00 H
ATOM 2661 2HG LYS A 335 19.683 34.841 7.632 1.00 0.00 H
ATOM 2662 1HD LYS A 335 21.680 33.321 7.738 1.00 0.00 H
ATOM 2663 2HD LYS A 335 21.599 33.409 9.514 1.00 0.00 H
ATOM 2664 1HE LYS A 335 19.225 32.548 9.361 1.00 0.00 H
ATOM 2665 2HE LYS A 335 19.502 32.280 7.623 1.00 0.00 H
ATOM 2666 1HZ LYS A 335 19.911 30.319 8.903 1.00 0.00 H
ATOM 2667 2HZ LYS A 335 21.309 30.840 8.200 1.00 0.00 H
ATOM 2668 3HZ LYS A 335 21.053 31.088 9.810 1.00 0.00 H
ATOM 2669 N ILE A 336 23.057 38.205 10.244 1.00 0.00 N
ATOM 2670 CA ILE A 336 23.633 39.538 10.190 1.00 0.00 C
ATOM 2671 C ILE A 336 24.018 39.940 11.605 1.00 0.00 C
ATOM 2672 O ILE A 336 23.314 39.621 12.558 1.00 0.00 O
ATOM 2673 CB ILE A 336 22.610 40.534 9.610 1.00 0.00 C
ATOM 2674 CGI ILE A 336 22.322 40.285 8.120 1.00 0.00 C
ATOM 2675 CG2 ILE A 336 23.039 41.995 9.828 1.00 0.00 C
ATOM 2676 CD1 ILE A 336 23.510 40.535 7.193 1.00 0.00 C
ATOM 2677 H ILE A 336 22.451 38.013 11.029 1.00 0.00 H
ATOM 2678 HA ILE A 336 24.508 39.531 9.540 1.00 0.00 H
ATOM 2679 HB ILE A 336 21.698 40.506 10.205 1.00 0.00 H

ATOM 2680 1HG1 ILE A 336 22.021 39.247 7.976 1.00 0.00 H
ATOM 2681 2HG1 ILE A 336 21.519 40.944 7.790 1.00 0.00 H
ATOM 2682 1HG2 ILE A 336 22.288 42.662 9.404 1.00 0.00 H
ATOM 2683 2HG2 ILE A 336 23.134 42.190 10.897 1.00 0.00 H
ATOM 2684 3HG2 ILE A 336 23.997 42.170 9.340 1.00 0.00 H
ATOM 2685 1HD1 ILE A 336 23.217 40.335 6.163 1.00 0.00 H
ATOM 2686 2HD1 ILE A 336 23.830 41.573 7.285 1.00 0.00 H
ATOM 2687 3HD1 ILE A 336 24.333 39.876 7.471 1.00 0.00 H
ATOM 2688 N GLY A 337 25.133 40.644 11.727 1.00 0.00 N
ATOM 2689 CA GLY A 337 25.565 41.309 12.934 1.00 0.00 C
ATOM 2690 C GLY A 337 26.341 42.534 12.477 1.00 0.00 C
ATOM 2691 O GLY A 337 26.918 42.512 11.390 1.00 0.00 O
ATOM 2692 H GLY A 337 25.755 40.746 10.938 1.00 0.00 H
ATOM 2693 1HA GLY A 337 24.694 41.592 13.526 1.00 0.00 H
ATOM 2694 2HA GLY A 337 26.195 40.636 13.515 1.00 0.00 H
ATOM 2695 N LEU A 338 26.313 43.619 13.239 1.00 0.00 N
ATOM 2696 CA LEU A 338 26.924 44.883 12.862 1.00 0.00 C
ATOM 2697 C LEU A 338 27.979 45.218 13.922 1.00 0.00 C
ATOM 2698 O LEU A 338 28.472 46.342 14.017 1.00 0.00 O
ATOM 2699 CB LEU A 338 25.818 45.939 12.702 1.00 0.00 C
ATOM 2700 CG LEU A 338 24.678 45.451 11.781 1.00 0.00 C
ATOM 2701 CD1 LEU A 338 23.457 46.360 11.883 1.00 0.00 C
ATOM 2702 CD2 LEU A 338 25.132 45.359 10.320 1.00 0.00 C
ATOM 2703 H LEU A 338 25.848 43.595 14.135 1.00 0.00 H
ATOM 2704 HA LEU A 338 27.316 44.810 11.848 1.00 0.00 H
ATOM 2705 1HB LEU A 338 25.390 46.168 13.678 1.00 0.00 H
ATOM 2706 2HB LEU A 338 26.240 46.846 12.269 1.00 0.00 H
ATOM 2707 HG LEU A 338 24.419 44.423 12.036 1.00 0.00 H
ATOM 2708 1HD1 LEU A 338 22.672 45.991 11.223 1.00 0.00 H
ATOM 2709 2HD1 LEU A 338 23.093 46.367 12.910 1.00 0.00 H
ATOM 2710 3HD1 LEU A 338 23.732 47.373 11.588 1.00 0.00 H
ATOM 2711 1HD2 LEU A 338 24.304 45.013 9.702 1.00 0.00 H
ATOM 2712 2HD2 LEU A 338 25.454 46.343 9.977 1.00 0.00 H
ATOM 2713 3HD2 LEU A 338 25.963 44.658 10.240 1.00 0.00 H
ATOM 2714 N ASP A 339 28.348 44.181 14.681 1.00 0.00 N
ATOM 2715 CA ASP A 339 29.134 44.181 15.900 1.00 0.00 C
ATOM 2716 C ASP A 339 30.447 44.930 15.679 1.00 0.00 C
ATOM 2717 O ASP A 339 31.018 45.515 16.596 1.00 0.00 O
ATOM 2718 CB ASP A 339 29.473 42.726 16.294 1.00 0.00 C
ATOM 2719 CG ASP A 339 28.328 41.725 16.238 1.00 0.00 C
ATOM 2720 OD1 ASP A 339 28.138 40.958 17.206 1.00 0.00 O
ATOM 2721 OD2 ASP A 339 27.684 41.582 15.174 1.00 0.00 Ol-
ATOM 2722 H ASP A 339 28.073 43.244 14.423 1.00 0.00 H
ATOM 2723 HA ASP A 339 28.582 44.691 16.689 1.00 0.00 H
ATOM 2724 1HB ASP A 339 30.242 42.337 15.625 1.00 0.00 H
ATOM 2725 2HB ASP A 339 29.840 42.703 17.320 1.00 0.00 H
ATOM 2726 N PHE A 340 30.971 44.822 14.456 1.00 0.00 N
ATOM 2727 CA PHE A 340 32.280 45.307 14.063 1.00 0.00 C
ATOM 2728 C PHE A 340 32.145 46.039 12.723 1.00 0.00 C
ATOM 2729 O PHE A 340 33.005 45.912 11.846 1.00 0.00 O
ATOM 2730 CB PHE A 340 33.253 44.115 13.954 1.00 0.00 C
ATOM 2731 CG PHE A 340 33.173 43.082 15.066 1.00 0.00 C
ATOM 2732 CD1 PHE A 340 33.279 43.462 16.418 1.00 0.00 C
ATOM 2733 CD2 PHE A 340 32.939 41.725 14.763 1.00 0.00 C
ATOM 2734 CE1 PHE A 340 33.072 42.525 17.445 1.00 0.00 C
ATOM 2735 CE2 PHE A 340 32.741 40.783 15.786 1.00 0.00 C
ATOM 2736 CZ PHE A 340 32.786 41.186 17.130 1.00 0.00 C
ATOM 2737 H PHE A 340 30.446 44.373 13.719 1.00 0.00 H
ATOM 2738 HA PHE A 340 32.670 45.969 14.836 1.00 0.00 H

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ATOM   2739 1HB  PHE A 340      33.064  43.575  13.026  1.00  0.00           H
ATOM   2740 2HB  PHE A 340      34.280  44.482  13.957  1.00  0.00           H
ATOM   2741  HD1 PHE A 340      33.522  44.483  16.674  1.00  0.00           H
ATOM   2742  HD2 PHE A 340      32.911  41.398  13.734  1.00  0.00           H
ATOM   2743  HE1 PHE A 340      33.132  42.833  18.478  1.00  0.00           H
ATOM   2744  HE2 PHE A 340      32.553  39.748  15.538  1.00  0.00           H
ATOM   2745  HZ  PHE A 340      32.602  40.473  17.920  1.00  0.00           H
ATOM   2746  N   CYS A 341      31.041  46.761  12.536  1.00  0.00           N
ATOM   2747  CA  CYS A 341      30.733  47.507  11.320  1.00  0.00           C
ATOM   2748  C   CYS A 341      31.140  48.962  11.550  1.00  0.00           C
ATOM   2749  O   CYS A 341      30.590  49.619  12.427  1.00  0.00           O
ATOM   2750  CB  CYS A 341      29.230  47.375  11.034  1.00  0.00           C
ATOM   2751  SG  CYS A 341      28.784  48.121   9.445  1.00  0.00           S
ATOM   2752  H   CYS A 341      30.346  46.820  13.266  1.00  0.00           H
ATOM   2753  HA  CYS A 341      31.274  47.073  10.480  1.00  0.00           H
ATOM   2754 1HB  CYS A 341      28.956  46.321  11.008  1.00  0.00           H
ATOM   2755 2HB  CYS A 341      28.665  47.877  11.820  1.00  0.00           H
ATOM   2756  HG  CYS A 341      27.703  48.007   9.276  1.00  0.00           H
ATOM   2757  N   LYS A 342      32.111  49.476  10.791  1.00  0.00           N
ATOM   2758  CA  LYS A 342      32.703  50.777  11.085  1.00  0.00           C
ATOM   2759  C   LYS A 342      31.913  51.913  10.437  1.00  0.00           C
ATOM   2760  O   LYS A 342      32.294  53.069  10.617  1.00  0.00           O
ATOM   2761  CB  LYS A 342      34.160  50.843  10.583  1.00  0.00           C
ATOM   2762  CG  LYS A 342      35.251  50.561  11.621  1.00  0.00           C
ATOM   2763  CD  LYS A 342      35.400  51.613  12.740  1.00  0.00           C
ATOM   2764  CE  LYS A 342      35.574  53.081  12.285  1.00  0.00           C
ATOM   2765  NZ  LYS A 342      34.307  53.852  12.236  1.00  0.00           N1+
ATOM   2766  H   LYS A 342      32.453  48.962   9.992  1.00  0.00           H
ATOM   2767  HA  LYS A 342      32.730  50.928  12.164  1.00  0.00           H
ATOM   2768 1HB  LYS A 342      34.305  50.108   9.791  1.00  0.00           H
ATOM   2769 2HB  LYS A 342      34.367  51.840  10.196  1.00  0.00           H
ATOM   2770 1HG  LYS A 342      35.045  49.614  12.119  1.00  0.00           H
ATOM   2771 2HG  LYS A 342      36.220  50.506  11.125  1.00  0.00           H
ATOM   2772 1HD  LYS A 342      34.512  51.599  13.372  1.00  0.00           H
ATOM   2773 2HD  LYS A 342      36.278  51.381  13.343  1.00  0.00           H
ATOM   2774 1HE  LYS A 342      36.239  53.600  12.975  1.00  0.00           H
ATOM   2775 2HE  LYS A 342      36.003  53.103  11.283  1.00  0.00           H
ATOM   2776 1HZ  LYS A 342      34.498  54.796  11.932  1.00  0.00           H
ATOM   2777 2HZ  LYS A 342      33.670  53.413  11.587  1.00  0.00           H
ATOM   2778 3HZ  LYS A 342      33.889  53.873  13.155  1.00  0.00           H
ATOM   2779  N   TYR A 343      30.891  51.620   9.636  1.00  0.00           N
ATOM   2780  CA  TYR A 343      30.311  52.594   8.722  1.00  0.00           C
ATOM   2781  C   TYR A 343      28.823  52.302   8.544  1.00  0.00           C
ATOM   2782  O   TYR A 343      28.446  51.144   8.356  1.00  0.00           O
ATOM   2783  CB  TYR A 343      31.050  52.517   7.377  1.00  0.00           C
ATOM   2784  CG  TYR A 343      32.508  52.914   7.469  1.00  0.00           C
ATOM   2785  CD1 TYR A 343      32.853  54.264   7.636  1.00  0.00           C
ATOM   2786  CD2 TYR A 343      33.533  51.950   7.456  1.00  0.00           C
ATOM   2787  CE1 TYR A 343      34.177  54.636   7.918  1.00  0.00           C
ATOM   2788  CE2 TYR A 343      34.863  52.322   7.716  1.00  0.00           C
ATOM   2789  CZ  TYR A 343      35.181  53.661   8.009  1.00  0.00           C
ATOM   2790  OH  TYR A 343      36.444  54.011  8.390  1.00  0.00           O
ATOM   2791  H   TYR A 343      30.490  50.693   9.648  1.00  0.00           H
ATOM   2792  HA  TYR A 343      30.461  53.599   9.118  1.00  0.00           H
ATOM   2793 1HB  TYR A 343      31.013  51.494   7.000  1.00  0.00           H
ATOM   2794 2HB  TYR A 343      30.574  53.185   6.660  1.00  0.00           H
ATOM   2795  HD1 TYR A 343      32.096  55.030   7.547  1.00  0.00           H
ATOM   2796  HD2 TYR A 343      33.299  50.916   7.245  1.00  0.00           H
ATOM   2797  HE1 TYR A 343      34.425  55.677   8.067  1.00  0.00           H
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ATOM   2798  HE2 TYR A 343      35.646  51.579   7.693  1.00  0.00           H
ATOM   2799  HH  TYR A 343      37.004  53.231   8.400  1.00  0.00           H
ATOM   2800  N   LEU A 344      27.995  53.343   8.606  1.00  0.00           N
ATOM   2801  CA  LEU A 344      26.551  53.265   8.476  1.00  0.00           C
ATOM   2802  C   LEU A 344      26.098  54.428   7.598  1.00  0.00           C
ATOM   2803  O   LEU A 344      26.349  55.582   7.942  1.00  0.00           O
ATOM   2804  CB  LEU A 344      25.914  53.364   9.868  1.00  0.00           C
ATOM   2805  CG  LEU A 344      24.396  53.616   9.825  1.00  0.00           C
ATOM   2806  CD1 LEU A 344      23.631  52.494   9.113  1.00  0.00           C
ATOM   2807  CD2 LEU A 344      23.877  53.746  11.256  1.00  0.00           C
ATOM   2808  H   LEU A 344      28.362  54.273   8.753  1.00  0.00           H
ATOM   2809  HA  LEU A 344      26.278  52.315   8.015  1.00  0.00           H
ATOM   2810  1HB LEU A 344      26.077  52.432  10.410  1.00  0.00           H
ATOM   2811  2HB LEU A 344      26.368  54.188  10.418  1.00  0.00           H
ATOM   2812  HG  LEU A 344      24.198  54.557   9.312  1.00  0.00           H
ATOM   2813  1HD1 LEU A 344      22.565  52.724   9.112  1.00  0.00           H
ATOM   2814  2HD1 LEU A 344      23.984  52.408   8.085  1.00  0.00           H
ATOM   2815  3HD1 LEU A 344      23.798  51.551  9.634  1.00  0.00           H
ATOM   2816  1HD2 LEU A 344      22.802  53.924  11.238  1.00  0.00           H
ATOM   2817  2HD2 LEU A 344      24.083  52.825  11.802  1.00  0.00           H
ATOM   2818  3HD2 LEU A 344      24.376  54.580  11.749  1.00  0.00           H
ATOM   2819  N   VAL A 345      25.407  54.126   6.501  1.00  0.00           N
ATOM   2820  CA  VAL A 345      24.861  55.116   5.587  1.00  0.00           C
ATOM   2821  C   VAL A 345      23.342  54.963   5.544  1.00  0.00           C
ATOM   2822  O   VAL A 345      22.829  53.847   5.632  1.00  0.00           O
ATOM   2823  CB  VAL A 345      25.437  54.907   4.179  1.00  0.00           C
ATOM   2824  CGI VAL A 345      24.920  55.965   3.195  1.00  0.00           C
ATOM   2825  CG2 VAL A 345      26.965  54.936   4.157  1.00  0.00           C
ATOM   2826  H   VAL A 345      25.234  53.159   6.263  1.00  0.00           H
ATOM   2827  HA  VAL A 345      25.122  56.115   5.935  1.00  0.00           H
ATOM   2828  HB  VAL A 345      25.180  53.909   3.825  1.00  0.00           H
ATOM   2829  1HG1 VAL A 345      25.350  55.785   2.209  1.00  0.00           H
ATOM   2830  2HG1 VAL A 345      23.834  55.905   3.134  1.00  0.00           H
ATOM   2831  3HG1 VAL A 345      25.210  56.957   3.541  1.00  0.00           H
ATOM   2832  1HG2 VAL A 345      27.316  54.784   3.136  1.00  0.00           H
ATOM   2833  2HG2 VAL A 345      27.316  55.902   4.521  1.00  0.00           H
ATOM   2834  3HG2 VAL A 345      27.353  54.144   4.796  1.00  0.00           H
ATOM   2835  N   LEU A 346      22.631  56.066   5.332  1.00  0.00           N
ATOM   2836  CA  LEU A 346      21.218  56.077   5.004  1.00  0.00           C
ATOM   2837  C   LEU A 346      21.062  57.021   3.805  1.00  0.00           C
ATOM   2838  O   LEU A 346      21.665  58.091   3.842  1.00  0.00           O
ATOM   2839  CB  LEU A 346      20.399  56.565   6.212  1.00  0.00           C
ATOM   2840  CG  LEU A 346      20.653  55.808   7.532  1.00  0.00           C
ATOM   2841  CD1 LEU A 346      21.776  56.432   8.375  1.00  0.00           C
ATOM   2842  CD2 LEU A 346      19.377  55.815   8.385  1.00  0.00           C
ATOM   2843  H   LEU A 346      23.073  56.972   5.395  1.00  0.00           H
ATOM   2844  HA  LEU A 346      20.892  55.065   4.762  1.00  0.00           H
ATOM   2845  1HB LEU A 346      20.629  57.613   6.408  1.00  0.00           H
ATOM   2846  2HB LEU A 346      19.336  56.462   5.997  1.00  0.00           H
ATOM   2847  HG  LEU A 346      20.939  54.779   7.312  1.00  0.00           H
ATOM   2848  1HD1 LEU A 346      21.908  55.856   9.290  1.00  0.00           H
ATOM   2849  2HD1 LEU A 346      22.705  56.426   7.805  1.00  0.00           H
ATOM   2850  3HD1 LEU A 346      21.513  57.459   8.628  1.00  0.00           H
ATOM   2851  1HD2 LEU A 346      19.559  55.279   9.317  1.00  0.00           H
ATOM   2852  2HD2 LEU A 346      19.094  56.844   8.607  1.00  0.00           H
ATOM   2853  3HD2 LEU A 346      18.571  55.327   7.837  1.00  0.00           H
ATOM   2854  N   ASP A 347      20.302  56.651   2.764  1.00  0.00           N
ATOM   2855  CA  ASP A 347      20.027  57.511   1.603  1.00  0.00           C
ATOM   2856  C   ASP A 347      18.540  57.443   1.239  1.00  0.00           C
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ATOM 2857 O ASP A 347 17.883 56.435 1.512 1.00 0.00 O
ATOM 2858 CB ASP A 347 20.924 57.169 0.397 1.00 0.00 C
ATOM 2859 CG ASP A 347 20.761 58.157 -0.757 1.00 0.00 C
ATOM 2860 OD1 ASP A 347 20.304 59.294 -0.522 1.00 0.00 O
ATOM 2861 OD2 ASP A 347 21.081 57.807 -1.914 1.00 0.00 Ol-
ATOM 2862 H ASP A 347 19.880 55.733 2.748 1.00 0.00 H
ATOM 2863 HA ASP A 347 20.371 58.524 1.812 1.00 0.00 H
ATOM 2864 1HB ASP A 347 21.970 57.185 0.704 1.00 0.00 H
ATOM 2865 2HB ASP A 347 20.670 56.176 0.025 1.00 0.00 H
ATOM 2866 N GLU A 348 18.029 58.539 0.665 1.00 0.00 N
ATOM 2867 CA GLU A 348 16.677 59.072 0.814 1.00 0.00 C
ATOM 2868 C GLU A 348 16.060 58.569 2.125 1.00 0.00 C
ATOM 2869 O GLU A 348 15.032 57.891 2.151 1.00 0.00 O
ATOM 2870 CB GLU A 348 15.835 58.944 -0.478 1.00 0.00 C
ATOM 2871 CG GLU A 348 16.692 59.452 -1.655 1.00 0.00 C
ATOM 2872 CD GLU A 348 16.012 59.946 -2.928 1.00 0.00 C
ATOM 2873 OE1 GLU A 348 14.773 59.879 -3.096 1.00 0.00 O
ATOM 2874 OE2 GLU A 348 16.816 60.418 -3.766 1.00 0.00 Ol-
ATOM 2875 H GLU A 348 18.600 59.099 0.049 1.00 0.00 H
ATOM 2876 HA GLU A 348 16.679 60.138 0.586 1.00 0.00 H
ATOM 2877 1HB GLU A 348 15.562 57.901 -0.633 1.00 0.00 H
ATOM 2878 2HB GLU A 348 14.930 59.546 -0.383 1.00 0.00 H
ATOM 2879 IHG GLU A 348 17.293 60.301 -1.328 1.00 0.00 H
ATOM 2880 2HG GLU A 348 17.349 58.653 -1.997 1.00 0.00 H
ATOM 2881 N ALA A 349 16.772 58.870 3.219 1.00 0.00 N
ATOM 2882 CA ALA A 349 16.468 58.374 4.548 1.00 0.00 C
ATOM 2883 C ALA A 349 15.187 59.003 5.076 1.00 0.00 C
ATOM 2884 O ALA A 349 14.519 58.439 5.938 1.00 0.00 O
ATOM 2885 CB ALA A 349 17.637 58.696 5.479 1.00 0.00 C
ATOM 2886 H ALA A 349 17.576 59.478 3.147 1.00 0.00 H
ATOM 2887 HA ALA A 349 16.363 57.289 4.516 1.00 0.00 H
ATOM 2888 1HB ALA A 349 17.416 58.327 6.481 1.00 0.00 H
ATOM 2889 2HB ALA A 349 18.542 58.217 5.106 1.00 0.00 H
ATOM 2890 3HB ALA A 349 17.786 59.775 5.515 1.00 0.00 H
ATOM 2891 N ASP A 350 14.893 60.189 4.559 1.00 0.00 N
ATOM 2892 CA ASP A 350 13.606 60.847 4.619 1.00 0.00 C
ATOM 2893 C ASP A 350 12.462 59.837 4.538 1.00 0.00 C
ATOM 2894 O ASP A 350 11.695 59.715 5.488 1.00 0.00 O
ATOM 2895 CB ASP A 350 13.549 61.908 3.520 1.00 0.00 C
ATOM 2896 CG ASP A 350 14.101 61.424 2.192 1.00 0.00 C
ATOM 2897 OD1 ASP A 350 13.371 60.708 1.478 1.00 0.00 O
ATOM 2898 OD2 ASP A 350 15.285 61.725 1.933 1.00 0.00 Ol-
ATOM 2899 H ASP A 350 15.602 60.717 4.069 1.00 0.00 H
ATOM 2900 HA ASP A 350 13.555 61.467 5.514 1.00 0.00 H
ATOM 2901 1HB ASP A 350 12.514 62.208 3.355 1.00 0.00 H
ATOM 2902 2HB ASP A 350 14.135 62.776 3.822 1.00 0.00 H
ATOM 2903 N ARG A 351 12.364 59.051 3.467 1.00 0.00 N
ATOM 2904 CA ARG A 351 11.253 58.118 3.312 1.00 0.00 C
ATOM 2905 C ARG A 351 11.480 56.808 4.071 1.00 0.00 C
ATOM 2906 O ARG A 351 10.882 55.783 3.748 1.00 0.00 O
ATOM 2907 CB ARG A 351 10.881 57.968 1.831 1.00 0.00 C
ATOM 2908 CG ARG A 351 9.653 57.104 1.499 1.00 0.00 C
ATOM 2909 CD ARG A 351 8.834 57.700 0.337 1.00 0.00 C
ATOM 2910 NE ARG A 351 7.925 58.767 0.804 1.00 0.00 N
ATOM 2911 CZ ARG A 351 7.275 59.688 0.071 1.00 0.00 C
ATOM 2912 NHl ARG A 351 6.411 60.496 0.663 1.00 0.00 N1+
ATOM 2913 NH2 ARG A 351 7.498 59.855 -1.230 1.00 0.00 N
ATOM 2914 H ARG A 351 13.066 59.094 2.742 1.00 0.00 H
ATOM 2915 HA ARG A 351 10.314 58.634 3.515 1.00 0.00 H

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ATOM   2916 1HB  ARG A 351     10.668  58.949   1.407  1.00  0.00          H
ATOM   2917 2HB  ARG A 351     11.711  57.512   1.291  1.00  0.00          H
ATOM   2918 1HG  ARG A 351      9.979  56.104   1.212  1.00  0.00          H
ATOM   2919 2HG  ARG A 351      9.008  57.038   2.375  1.00  0.00          H
ATOM   2920 1HD  ARG A 351      9.511  58.125  -0.405  1.00  0.00          H
ATOM   2921 2HD  ARG A 351      8.235  56.916  -0.125  1.00  0.00          H
ATOM   2922  HE  ARG A 351      7.817  58.753   1.808  1.00  0.00          H
ATOM   2923 1HH1 ARG A 351      5.917  61.191   0.122  1.00  0.00          H
ATOM   2924 2HH1 ARG A 351      6.244  60.417   1.656  1.00  0.00          H
ATOM   2925 1HH2 ARG A 351      6.988  60.559  -1.744  1.00  0.00          H
ATOM   2926 2HH2 ARG A 351      8.178  59.278  -1.704  1.00  0.00          H
ATOM   2927  N   MET A 352     12.295  56.841   5.127  1.00  0.00          N
ATOM   2928  CA  MET A 352     12.257  55.874   6.212  1.00  0.00          C
ATOM   2929  C   MET A 352     11.695  56.549   7.468  1.00  0.00          C
ATOM   2930  O   MET A 352     11.638  55.932   8.529  1.00  0.00          O
ATOM   2931  CB  MET A 352     13.658  55.294   6.452  1.00  0.00          C
ATOM   2932  CG  MET A 352     14.188  54.633   5.177  1.00  0.00          C
ATOM   2933  SD  MET A 352     15.628  53.552   5.395  1.00  0.00          S
ATOM   2934  CE  MET A 352     16.958  54.776   5.396  1.00  0.00          C
ATOM   2935  H   MET A 352     12.991  57.569   5.205  1.00  0.00          H
ATOM   2936  HA  MET A 352     11.666  55.010   5.909  1.00  0.00          H
ATOM   2937 1HB  MET A 352     14.338  56.093   6.745  1.00  0.00          H
ATOM   2938 2HB  MET A 352     13.612  54.547   7.245  1.00  0.00          H
ATOM   2939 1HG  MET A 352     13.407  54.016   4.735  1.00  0.00          H
ATOM   2940 2HG  MET A 352     14.489  55.403   4.467  1.00  0.00          H
ATOM   2941 1HE  MET A 352     17.916  54.272   5.522  1.00  0.00          H
ATOM   2942 2HE  MET A 352     16.954  55.318   4.451  1.00  0.00          H
ATOM   2943 3HE  MET A 352     16.807  55.477   6.217  1.00  0.00          H
ATOM   2944  N   LEU A 353     11.277  57.808   7.342  1.00  0.00          N
ATOM   2945  CA  LEU A 353     10.646  58.622   8.365  1.00  0.00          C
ATOM   2946  C   LEU A 353      9.255  59.017   7.868  1.00  0.00          C
ATOM   2947  O   LEU A 353      8.318  58.993   8.663  1.00  0.00          O
ATOM   2948  CB  LEU A 353     11.490  59.857   8.713  1.00  0.00          C
ATOM   2949  CG  LEU A 353     12.935  59.523   9.121  1.00  0.00          C
ATOM   2950  CD1 LEU A 353     13.710  60.825   9.340  1.00  0.00          C
ATOM   2951  CD2 LEU A 353     13.002  58.684  10.404  1.00  0.00          C
ATOM   2952  H   LEU A 353     11.387  58.291   6.462  1.00  0.00          H
ATOM   2953  HA  LEU A 353     10.614  58.067   9.303  1.00  0.00          H
ATOM   2954 1HB  LEU A 353     11.542  60.517   7.847  1.00  0.00          H
ATOM   2955 2HB  LEU A 353     11.032  60.388   9.547  1.00  0.00          H
ATOM   2956  HG  LEU A 353     13.406  58.928   8.338  1.00  0.00          H
ATOM   2957 1HD1 LEU A 353     14.735  60.595   9.630  1.00  0.00          H
ATOM   2958 2HD1 LEU A 353     13.716  61.405   8.417  1.00  0.00          H
ATOM   2959 3HD1 LEU A 353     13.232  61.405  10.129  1.00  0.00          H
ATOM   2960 1HD2 LEU A 353     14.043  58.476  10.648  1.00  0.00          H
ATOM   2961 2HD2 LEU A 353     12.540  59.235  11.223  1.00  0.00          H
ATOM   2962 3HD2 LEU A 353     12.470  57.745  10.252  1.00  0.00          H
ATOM   2963  N   ASP A 354      9.083  59.257   6.556  1.00  0.00          N
ATOM   2964  CA  ASP A 354      7.757  59.390   5.938  1.00  0.00          C
ATOM   2965  C   ASP A 354      6.879  58.188   6.320  1.00  0.00          C
ATOM   2966  O   ASP A 354      5.656  58.250   6.230  1.00  0.00          O
ATOM   2967  CB  ASP A 354      7.800  59.387   4.393  1.00  0.00          C
ATOM   2968  CG  ASP A 354      8.392  60.599   3.687  1.00  0.00          C
ATOM   2969  OD1 ASP A 354      9.587  60.892   3.863  1.00  0.00          O
ATOM   2970  OD2 ASP A 354      7.704  61.134   2.795  1.00  0.00          Ol-
ATOM   2971  H   ASP A 354      9.885  59.353   5.950  1.00  0.00          H
ATOM   2972  HA  ASP A 354      7.264  60.283   6.323  1.00  0.00          H
ATOM   2973 1HB  ASP A 354      8.395  58.541   4.047  1.00  0.00          H
ATOM   2974 2HB  ASP A 354      6.786  59.301   4.001  1.00  0.00          H
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ATOM 2975 N MET A 355 7.512 57.051 6.628 1.00 0.00 N
ATOM 2976 CA MET A 355 6.861 55.786 6.933 1.00 0.00 C
ATOM 2977 C MET A 355 7.316 55.281 8.308 1.00 0.00 C
ATOM 2978 O MET A 355 7.150 54.107 8.627 1.00 0.00 O
ATOM 2979 CB MET A 355 7.191 54.774 5.827 1.00 0.00 C
ATOM 2980 CG MET A 355 6.792 55.283 4.435 1.00 0.00 C
ATOM 2981 SD MET A 355 7.130 54.142 3.065 1.00 0.00 S
ATOM 2982 CE MET A 355 5.912 52.842 3.398 1.00 0.00 C
ATOM 2983 H MET A 355 8.521 57.028 6.661 1.00 0.00 H
ATOM 2984 HA MET A 355 5.779 55.916 6.900 1.00 0.00 H
ATOM 2985 1HB MET A 355 8.263 54.579 5.820 1.00 0.00 H
ATOM 2986 2HB MET A 355 6.654 53.844 6.013 1.00 0.00 H
ATOM 2987 1HG MET A 355 5.720 55.482 4.414 1.00 0.00 H
ATOM 2988 2HG MET A 355 7.336 56.201 4.214 1.00 0.00 H
ATOM 2989 1HE MET A 355 5.994 52.064 2.640 1.00 0.00 H
ATOM 2990 2HE MET A 355 6.100 52.411 4.382 1.00 0.00 H
ATOM 2991 3HE MET A 355 4.909 53.268 3.375 1.00 0.00 H
ATOM 2992 N GLY A 356 7.888 56.179 9.113 1.00 0.00 N
ATOM 2993 CA GLY A 356 8.304 55.964 10.491 1.00 0.00 C
ATOM 2994 C GLY A 356 8.948 54.600 10.765 1.00 0.00 C
ATOM 2995 O GLY A 356 8.502 53.867 11.649 1.00 0.00 O
ATOM 2996 H GLY A 356 8.070 57.114 8.778 1.00 0.00 H
ATOM 2997 1HA GLY A 356 9.038 56.719 10.771 1.00 0.00 H
ATOM 2998 2HA GLY A 356 7.437 56.038 11.148 1.00 0.00 H
ATOM 2999 N PHE A 357 10.059 54.285 10.095 1.00 0.00 N
ATOM 3000 CA PHE A 357 10.764 53.026 10.303 1.00 0.00 C
ATOM 3001 C PHE A 357 11.683 53.096 11.529 1.00 0.00 C
ATOM 3002 O PHE A 357 12.416 52.142 11.788 1.00 0.00 O
ATOM 3003 CB PHE A 357 11.586 52.633 9.063 1.00 0.00 C
ATOM 3004 CG PHE A 357 10.851 52.353 7.762 1.00 0.00 C
ATOM 3005 CD1 PHE A 357 9.461 52.125 7.717 1.00 0.00 C
ATOM 3006 CD2 PHE A 357 11.578 52.296 6.556 1.00 0.00 C
ATOM 3007 CE1 PHE A 357 8.814 51.861 6.499 1.00 0.00 C
ATOM 3008 CE2 PHE A 357 10.933 52.047 5.331 1.00 0.00 C
ATOM 3009 CZ PHE A 357 9.547 51.830 5.301 1.00 0.00 C
ATOM 3010 H PHE A 357 10.440 54.929 9.416 1.00 0.00 H
ATOM 3011 HA PHE A 357 10.042 52.217 10.408 1.00 0.00 H
ATOM 3012 1HB PHE A 357 12.284 53.434 8.820 1.00 0.00 H
ATOM 3013 2HB PHE A 357 12.141 51.718 9.270 1.00 0.00 H
ATOM 3014 HD1 PHE A 357 8.880 52.152 8.627 1.00 0.00 H
ATOM 3015 HD2 PHE A 357 12.648 52.446 6.563 1.00 0.00 H
ATOM 3016 HE1 PHE A 357 7.749 51.681 6.480 1.00 0.00 H
ATOM 3017 HE2 PHE A 357 11.504 52.022 4.415 1.00 0.00 H
ATOM 3018 HZ PHE A 357 9.043 51.641 4.365 1.00 0.00 H
ATOM 3019 N GLU A 358 11.679 54.215 12.259 1.00 0.00 N
ATOM 3020 CA GLU A 358 12.470 54.436 13.465 1.00 0.00 C
ATOM 3021 C GLU A 358 12.538 53.195 14.376 1.00 0.00 C
ATOM 3022 O GLU A 358 13.627 52.814 14.806 1.00 0.00 O
ATOM 3023 CB GLU A 358 11.978 55.693 14.204 1.00 0.00 C
ATOM 3024 CG GLU A 358 12.836 56.921 13.874 1.00 0.00 C
ATOM 3025 CD GLU A 358 14.110 56.912 14.701 1.00 0.00 C
ATOM 3026 OE1 GLU A 358 14.998 56.088 14.408 1.00 0.00 O
ATOM 3027 OE2 GLU A 358 14.170 57.667 15.693 1.00 0.00 Ol-
ATOM 3028 H GLU A 358 11.095 54.993 11.987 1.00 0.00 H
ATOM 3029 HA GLU A 358 13.451 54.825 13.191 1.00 0.00 H
ATOM 3030 1HB GLU A 358 10.949 55.907 13.914 1.00 0.00 H
ATOM 3031 2HB GLU A 358 12.024 55.524 15.280 1.00 0.00 H
ATOM 3032 1HG GLU A 358 13.098 56.908 12.816 1.00 0.00 H
ATOM 3033 2HG GLU A 358 12.274 57.828 14.097 1.00 0.00 H

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ATOM   3034  N   PRO A 359      11.425  52.494  14.654  1.00  0.00           N
ATOM   3035  CA  PRO A 359      11.476  51.384  15.592  1.00  0.00           C
ATOM   3036  C   PRO A 359      12.271  50.196  15.033  1.00  0.00           C
ATOM   3037  O   PRO A 359      12.624  49.279  15.771  1.00  0.00           O
ATOM   3038  CB  PRO A 359      10.018  51.013  15.880  1.00  0.00           C
ATOM   3039  CG  PRO A 359      9.272  52.324  15.625  1.00  0.00           C
ATOM   3040  CD  PRO A 359      10.054  52.944  14.468  1.00  0.00           C
ATOM   3041  HA  PRO A 359      11.918  51.720  16.530  1.00  0.00           H
ATOM   3042  1HB PRO A 359      9.705  50.216  15.206  1.00  0.00           H
ATOM   3043  2HB PRO A 359      9.926  50.673  16.912  1.00  0.00           H
ATOM   3044  1HG PRO A 359      8.236  52.108  15.363  1.00  0.00           H
ATOM   3045  2HG PRO A 359      9.298  52.939  16.525  1.00  0.00           H
ATOM   3046  1HD PRO A 359      10.021  54.033  14.499  1.00  0.00           H
ATOM   3047  2HD PRO A 359      9.685  52.597  13.503  1.00  0.00           H
ATOM   3048  N   GLN A 360      12.545  50.203  13.727  1.00  0.00           N
ATOM   3049  CA  GLN A 360      13.457  49.273  13.093  1.00  0.00           C
ATOM   3050  C   GLN A 360      14.850  49.894  12.992  1.00  0.00           C
ATOM   3051  O   GLN A 360      15.835  49.180  13.148  1.00  0.00           O
ATOM   3052  CB  GLN A 360      12.962  48.852  11.705  1.00  0.00           C
ATOM   3053  CG  GLN A 360      11.522  48.326  11.743  1.00  0.00           C
ATOM   3054  CD  GLN A 360      10.537  49.380  11.259  1.00  0.00           C
ATOM   3055  NE2 GLN A 360      9.891  50.096  12.168  1.00  0.00           N
ATOM   3056  OE1 GLN A 360      10.371  49.553  10.058  1.00  0.00           O
ATOM   3057  H   GLN A 360      12.106  50.884  13.123  1.00  0.00           H
ATOM   3058  HA  GLN A 360      13.477  48.341  13.658  1.00  0.00           H
ATOM   3059  1HB GLN A 360      12.992  49.710  11.033  1.00  0.00           H
ATOM   3060  2HB GLN A 360      13.602  48.062  11.314  1.00  0.00           H
ATOM   3061  1HG GLN A 360      11.438  47.450  11.100  1.00  0.00           H
ATOM   3062  2HG GLN A 360      11.262  48.052  12.765  1.00  0.00           H
ATOM   3063  1HE2 GLN A 360     9.231  50.803  11.878  1.00  0.00           H
ATOM   3064  2HE2 GLN A 360     10.060  49.934  13.151  1.00  0.00           H
ATOM   3065  N   ILE A 361      14.949  51.190  12.688  1.00  0.00           N
ATOM   3066  CA  ILE A 361      16.239  51.850  12.536  1.00  0.00           C
ATOM   3067  C   ILE A 361      17.000  51.782  13.860  1.00  0.00           C
ATOM   3068  O   ILE A 361      18.152  51.360  13.884  1.00  0.00           O
ATOM   3069  CB  ILE A 361      16.115  53.295  12.012  1.00  0.00           C
ATOM   3070  CGI ILE A 361      15.418  53.341  10.639  1.00  0.00           C
ATOM   3071  CG2 ILE A 361      17.512  53.922  11.876  1.00  0.00           C
ATOM   3072  CD1 ILE A 361      15.024  54.766  10.232  1.00  0.00           C
ATOM   3073  H   ILE A 361      14.115  51.744  12.557  1.00  0.00           H
ATOM   3074  HA  ILE A 361      16.776  51.410  11.695  1.00  0.00           H
ATOM   3075  HB  ILE A 361      15.538  53.890  12.720  1.00  0.00           H
ATOM   3076  1HG1 ILE A 361     16.090  52.948  9.876  1.00  0.00           H
ATOM   3077  2HG1 ILE A 361     14.511  52.738  10.670  1.00  0.00           H
ATOM   3078  1HG2 ILE A 361     17.418  54.943  11.506  1.00  0.00           H
ATOM   3079  2HG2 ILE A 361     18.002  53.933  12.850  1.00  0.00           H
ATOM   3080  3HG2 ILE A 361     18.108  53.336  11.177  1.00  0.00           H
ATOM   3081  1HD1 ILE A 361     14.537  54.745  9.257  1.00  0.00           H
ATOM   3082  2HD1 ILE A 361     14.338  55.179  10.972  1.00  0.00           H
ATOM   3083  3HD1 ILE A 361     15.917  55.389  10.178  1.00  0.00           H
ATOM   3084  N   ARG A 362      16.385  52.179  14.972  1.00  0.00           N
ATOM   3085  CA  ARG A 362      17.072  52.146  16.256  1.00  0.00           C
ATOM   3086  C   ARG A 362      17.515  50.714  16.557  1.00  0.00           C
ATOM   3087  O   ARG A 362      18.610  50.486  17.067  1.00  0.00           O
ATOM   3088  CB  ARG A 362      16.167  52.673  17.375  1.00  0.00           C
ATOM   3089  CG  ARG A 362      15.727  54.125  17.169  1.00  0.00           C
ATOM   3090  CD  ARG A 362      16.871  55.136  17.304  1.00  0.00           C
ATOM   3091  NE  ARG A 362      16.352  56.475  17.006  1.00  0.00           N
ATOM   3092  CZ  ARG A 362      16.677  57.622  17.608  1.00  0.00           C
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ATOM   3093  NH1 ARG A 362      17.749  57.714  18.389  1.00  0.00      N1+
ATOM   3094  NH2 ARG A 362      15.898  58.678  17.436  1.00  0.00      N
ATOM   3095  H   ARG A 362      15.431  52.508  14.932  1.00  0.00      H
ATOM   3096  HA  ARG A 362      17.923  52.826  16.231  1.00  0.00      H
ATOM   3097  1HB ARG A 362      15.266  52.062  17.432  1.00  0.00      H
ATOM   3098  2HB ARG A 362      16.699  52.624  18.325  1.00  0.00      H
ATOM   3099  1HG ARG A 362      15.307  54.239  16.169  1.00  0.00      H
ATOM   3100  2HG ARG A 362      14.972  54.385  17.911  1.00  0.00      H
ATOM   3101  1HD ARG A 362      17.262  55.109  18.321  1.00  0.00      H
ATOM   3102  2HD ARG A 362      17.665  54.883  16.603  1.00  0.00      H
ATOM   3103  HE  ARG A 362      15.678  56.472  16.254  1.00  0.00      H
ATOM   3104  1HH1 ARG A 362     17.975  58.592  18.834  1.00  0.00      H
ATOM   3105  2HH1 ARG A 362     18.337  56.907  18.537  1.00  0.00      H
ATOM   3106  1HH2 ARG A 362     16.129  59.554  17.884  1.00  0.00      H
ATOM   3107  2HH2 ARG A 362     15.074  58.609  16.857  1.00  0.00      H
ATOM   3108  N   ARG A 363      16.676  49.750  16.177  1.00  0.00      N
ATOM   3109  CA  ARG A 363      16.873  48.321  16.378  1.00  0.00      C
ATOM   3110  C   ARG A 363      17.874  47.754  15.355  1.00  0.00      C
ATOM   3111  O   ARG A 363      18.016  46.543  15.204  1.00  0.00      O
ATOM   3112  CB  ARG A 363      15.477  47.664  16.344  1.00  0.00      C
ATOM   3113  CG  ARG A 363      15.376  46.138  16.489  1.00  0.00      C
ATOM   3114  CD  ARG A 363      15.956  45.585  17.802  1.00  0.00      C
ATOM   3115  NE  ARG A 363      16.689  44.328  17.587  1.00  0.00      N
ATOM   3116  CZ  ARG A 363      16.193  43.181  17.123  1.00  0.00      C
ATOM   3117  NH1 ARG A 363      14.880  43.061  16.922  1.00  0.00      N1+
ATOM   3118  NH2 ARG A 363      17.033  42.187  16.865  1.00  0.00      N
ATOM   3119  H   ARG A 363      15.814  49.987  15.706  1.00  0.00      H
ATOM   3120  HA  ARG A 363      17.164  48.136  17.412  1.00  0.00      H
ATOM   3121  1HB ARG A 363      14.869  48.059  17.158  1.00  0.00      H
ATOM   3122  2HB ARG A 363      14.995  47.884  15.392  1.00  0.00      H
ATOM   3123  1HG ARG A 363      14.329  45.838  16.452  1.00  0.00      H
ATOM   3124  2HG ARG A 363      15.920  45.659  15.674  1.00  0.00      H
ATOM   3125  1HD ARG A 363      16.643  46.313  18.232  1.00  0.00      H
ATOM   3126  2HD ARG A 363      15.145  45.393  18.505  1.00  0.00      H
ATOM   3127  HE  ARG A 363      17.667  44.393  17.832  1.00  0.00      H
ATOM   3128  1HH1 ARG A 363     14.500  42.194  16.570  1.00  0.00      H
ATOM   3129  2HH1 ARG A 363     14.266  43.838  17.121  1.00  0.00      H
ATOM   3130  1HH2 ARG A 363     16.683  41.308  16.513  1.00  0.00      H
ATOM   3131  2HH2 ARG A 363     18.024  42.310  17.021  1.00  0.00      H
ATOM   3132  N   ILE A 364      18.590  48.629  14.653  1.00  0.00      N
ATOM   3133  CA  ILE A 364      19.730  48.312  13.817  1.00  0.00      C
ATOM   3134  C   ILE A 364      20.906  49.146  14.315  1.00  0.00      C
ATOM   3135  O   ILE A 364      22.031  48.660  14.389  1.00  0.00      O
ATOM   3136  CB  ILE A 364      19.398  48.646  12.349  1.00  0.00      C
ATOM   3137  CGI ILE A 364      18.377  47.641  11.796  1.00  0.00      C
ATOM   3138  CG2 ILE A 364      20.656  48.692  11.471  1.00  0.00      C
ATOM   3139  CD1 ILE A 364      17.721  48.163  10.516  1.00  0.00      C
ATOM   3140  H   ILE A 364      18.352  49.611  14.677  1.00  0.00      H
ATOM   3141  HA  ILE A 364      19.948  47.247  13.888  1.00  0.00      H
ATOM   3142  HB  ILE A 364      19.045  49.675  12.281  1.00  0.00      H
ATOM   3143  1HG1 ILE A 364     18.879  46.701  11.569  1.00  0.00      H
ATOM   3144  2HG1 ILE A 364     17.599  47.467  12.538  1.00  0.00      H
ATOM   3145  1HG2 ILE A 364     20.376  48.931  10.445  1.00  0.00      H
ATOM   3146  2HG2 ILE A 364     21.336  49.456  11.848  1.00  0.00      H
ATOM   3147  3HG2 ILE A 364     21.152  47.721  11.495  1.00  0.00      H
ATOM   3148  1HD1 ILE A 364     17.003  47.429  10.149  1.00  0.00      H
ATOM   3149  2HD1 ILE A 364     17.205  49.100  10.728  1.00  0.00      H
ATOM   3150  3HD1 ILE A 364     18.485  48.334  9.758  1.00  0.00      H
ATOM   3151  N   VAL A 365      20.655  50.428  14.560  1.00  0.00      N
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ATOM 3152 CA VAL A 365 21.681 51.448 14.570 1.00 0.00 C
ATOM 3153 C VAL A 365 22.255 51.656 15.973 1.00 0.00 C
ATOM 3154 O VAL A 365 23.406 52.085 16.087 1.00 0.00 O
ATOM 3155 CB VAL A 365 21.093 52.727 13.933 1.00 0.00 C
ATOM 3156 CGI VAL A 365 22.007 53.949 14.066 1.00 0.00 C
ATOM 3157 CG2 VAL A 365 20.812 52.481 12.441 1.00 0.00 C
ATOM 3158 H VAL A 365 19.711 50.731 14.751 1.00 0.00 H
ATOM 3159 HA VAL A 365 22.439 51.209 13.824 1.00 0.00 H
ATOM 3160 HB VAL A 365 20.132 52.954 14.393 1.00 0.00 H
ATOM 3161 1HG1 VAL A 365 21.532 54.811 13.597 1.00 0.00 H
ATOM 3162 2HG1 VAL A 365 22.181 54.160 15.121 1.00 0.00 H
ATOM 3163 3HG1 VAL A 365 22.958 53.747 13.575 1.00 0.00 H
ATOM 3164 1HG2 VAL A 365 20.397 53.385 11.995 1.00 0.00 H
ATOM 3165 2HG2 VAL A 365 21.741 52.219 11.934 1.00 0.00 H
ATOM 3166 3HG2 VAL A 365 20.098 51.664 12.336 1.00 0.00 H
ATOM 3167 N GLU A 366 21.475 51.407 17.030 1.00 0.00 N
ATOM 3168 CA GLU A 366 21.892 51.754 18.384 1.00 0.00 C
ATOM 3169 C GLU A 366 21.170 50.949 19.472 1.00 0.00 C
ATOM 3170 O GLU A 366 21.348 51.222 20.658 1.00 0.00 O
ATOM 3171 CB GLU A 366 21.800 53.281 18.601 1.00 0.00 C
ATOM 3172 CG GLU A 366 20.691 54.017 17.817 1.00 0.00 C
ATOM 3173 CD GLU A 366 20.937 55.516 17.727 1.00 0.00 C
ATOM 3174 OE1 GLU A 366 19.979 56.257 18.027 1.00 0.00 O
ATOM 3175 OE2 GLU A 366 22.066 55.893 17.325 1.00 0.00 Ol-
ATOM 3176 H GLU A 366 20.575 50.968 16.901 1.00 0.00 H
ATOM 3177 HA GLU A 366 22.979 51.705 18.454 1.00 0.00 H
ATOM 3178 1HB GLU A 366 21.611 53.489 19.654 1.00 0.00 H
ATOM 3179 2HB GLU A 366 22.738 53.749 18.302 1.00 0.00 H
ATOM 3180 1HG GLU A 366 20.641 53.624 16.801 1.00 0.00 H
ATOM 3181 2HG GLU A 366 19.732 53.864 18.313 1.00 0.00 H
ATOM 3182 N GLN A 367 20.351 49.966 19.100 1.00 0.00 N
ATOM 3183 CA GLN A 367 19.615 49.130 20.038 1.00 0.00 C
ATOM 3184 C GLN A 367 19.646 47.681 19.547 1.00 0.00 C
ATOM 3185 O GLN A 367 18.634 46.985 19.551 1.00 0.00 O
ATOM 3186 CB GLN A 367 18.181 49.651 20.222 1.00 0.00 C
ATOM 3187 CG GLN A 367 18.148 51.124 20.655 1.00 0.00 C
ATOM 3188 CD GLN A 367 16.731 51.618 20.909 1.00 0.00 C
ATOM 3189 NE2 GLN A 367 16.571 52.919 21.116 1.00 0.00 N
ATOM 3190 OE1 GLN A 367 15.777 50.850 20.905 1.00 0.00 O
ATOM 3191 H GLN A 367 20.215 49.766 18.120 1.00 0.00 H
ATOM 3192 HA GLN A 367 20.034 49.248 21.038 1.00 0.00 H
ATOM 3193 1HB GLN A 367 17.639 49.564 19.281 1.00 0.00 H
ATOM 3194 2HB GLN A 367 17.675 49.063 20.988 1.00 0.00 H
ATOM 3195 1HG GLN A 367 18.718 51.245 21.576 1.00 0.00 H
ATOM 3196 2HG GLN A 367 18.587 51.743 19.873 1.00 0.00 H
ATOM 3197 1HE2 GLN A 367 15.649 53.292 21.289 1.00 0.00 H
ATOM 3198 2HE2 GLN A 367 17.371 53.535 21.101 1.00 0.00 H
ATOM 3199 N ASP A 368 20.839 47.234 19.155 1.00 0.00 N
ATOM 3200 CA ASP A 368 21.197 45.852 18.852 1.00 0.00 C
ATOM 3201 C ASP A 368 22.730 45.840 18.788 1.00 0.00 C
ATOM 3202 O ASP A 368 23.364 46.769 19.292 1.00 0.00 O
ATOM 3203 CB ASP A 368 20.551 45.362 17.545 1.00 0.00 C
ATOM 3204 CG ASP A 368 20.405 43.845 17.508 1.00 0.00 C
ATOM 3205 OD1 ASP A 368 21.432 43.157 17.336 1.00 0.00 O
ATOM 3206 OD2 ASP A 368 19.252 43.372 17.620 1.00 0.00 Ol-
ATOM 3207 H ASP A 368 21.608 47.879 19.042 1.00 0.00 H
ATOM 3208 HA ASP A 368 20.787 45.194 19.618 1.00 0.00 H
ATOM 3209 1HB ASP A 368 19.558 45.799 17.443 1.00 0.00 H
ATOM 3210 2HB ASP A 368 21.169 45.662 16.699 1.00 0.00 H

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ATOM   3211 N   THR A 369     23.357  44.846  18.166  1.00  0.00      N
ATOM   3212 CA  THR A 369     24.806  44.766  18.132  1.00  0.00      C
ATOM   3213 C   THR A 369     25.354  45.662  17.007  1.00  0.00      C
ATOM   3214 O   THR A 369     25.684  45.192  15.916  1.00  0.00      O
ATOM   3215 CB  THR A 369     25.260  43.288  18.114  1.00  0.00      C
ATOM   3216 CG2 THR A 369     24.861  42.486  16.868  1.00  0.00      C
ATOM   3217 OG1 THR A 369     26.659  43.180  18.325  1.00  0.00      O
ATOM   3218 H   THR A 369     22.825  44.124  17.702  1.00  0.00      H
ATOM   3219 HA  THR A 369     25.203  44.937  19.132  1.00  0.00      H
ATOM   3220 HB  THR A 369     24.915  42.790  19.020  1.00  0.00      H
ATOM   3221 1HG2 THR A 369     25.230  41.464  16.960  1.00  0.00      H
ATOM   3222 2HG2 THR A 369     23.775  42.473  16.776  1.00  0.00      H
ATOM   3223 3HG2 THR A 369     25.295  42.950  15.982  1.00  0.00      H
ATOM   3224 HG1 THR A 369     26.916  42.255  18.309  1.00  0.00      H
ATOM   3225 N   MET A 370     25.509  46.955  17.307  1.00  0.00      N
ATOM   3226 CA  MET A 370     26.251  47.921  16.512  1.00  0.00      C
ATOM   3227 C   MET A 370     26.904  48.917  17.478  1.00  0.00      C
ATOM   3228 O   MET A 370     26.235  49.410  18.383  1.00  0.00      O
ATOM   3229 CB  MET A 370     25.340  48.677  15.531  1.00  0.00      C
ATOM   3230 CG  MET A 370     26.209  49.497  14.560  1.00  0.00      C
ATOM   3231 SD  MET A 370     25.369  50.740  13.550  1.00  0.00      S
ATOM   3232 CE  MET A 370     24.560  49.685  12.333  1.00  0.00      C
ATOM   3233 H   MET A 370     25.092  47.332  18.146  1.00  0.00      H
ATOM   3234 HA  MET A 370     27.009  47.402  15.924  1.00  0.00      H
ATOM   3235 1HB  MET A 370     24.738  47.964  14.969  1.00  0.00      H
ATOM   3236 2HB  MET A 370     24.683  49.347  16.087  1.00  0.00      H
ATOM   3237 1HG  MET A 370     26.967  50.042  15.123  1.00  0.00      H
ATOM   3238 2HG  MET A 370     26.696  48.826  13.853  1.00  0.00      H
ATOM   3239 1HE  MET A 370     23.997  50.303  11.633  1.00  0.00      H
ATOM   3240 2HE  MET A 370     25.312  49.114  11.790  1.00  0.00      H
ATOM   3241 3HE  MET A 370     23.881  49.000  12.840  1.00  0.00      H
ATOM   3242 N   PRO A 371     28.191  49.248  17.309  1.00  0.00      N
ATOM   3243 CA  PRO A 371     28.809  50.328  18.063  1.00  0.00      C
ATOM   3244 C   PRO A 371     28.146  51.693  17.783  1.00  0.00      C
ATOM   3245 O   PRO A 371     27.597  51.896  16.702  1.00  0.00      O
ATOM   3246 CB  PRO A 371     30.267  50.336  17.595  1.00  0.00      C
ATOM   3247 CG  PRO A 371     30.520  48.905  17.120  1.00  0.00      C
ATOM   3248 CD  PRO A 371     29.169  48.511  16.530  1.00  0.00      C
ATOM   3249 HA  PRO A 371     28.717  50.126  19.130  1.00  0.00      H
ATOM   3250 1HB  PRO A 371     30.387  51.060  16.790  1.00  0.00      H
ATOM   3251 2HB  PRO A 371     30.915  50.609  18.429  1.00  0.00      H
ATOM   3252 1HG  PRO A 371     31.321  48.904  16.381  1.00  0.00      H
ATOM   3253 2HG  PRO A 371     30.808  48.286  17.969  1.00  0.00      H
ATOM   3254 1HD  PRO A 371     28.983  47.442  16.631  1.00  0.00      H
ATOM   3255 2HD  PRO A 371     29.089  48.796  15.481  1.00  0.00      H
ATOM   3256 N   PRO A 372     28.239  52.662  18.704  1.00  0.00      N
ATOM   3257 CA  PRO A 372     27.552  53.941  18.564  1.00  0.00      C
ATOM   3258 C   PRO A 372     28.309  54.890  17.620  1.00  0.00      C
ATOM   3259 O   PRO A 372     29.373  54.544  17.105  1.00  0.00      O
ATOM   3260 CB  PRO A 372     27.479  54.503  19.989  1.00  0.00      C
ATOM   3261 CG  PRO A 372     28.706  53.897  20.669  1.00  0.00      C
ATOM   3262 CD  PRO A 372     28.770  52.505  20.045  1.00  0.00      C
ATOM   3263 HA  PRO A 372     26.549  53.774  18.172  1.00  0.00      H
ATOM   3264 1HB  PRO A 372     27.517  55.591  19.953  1.00  0.00      H
ATOM   3265 2HB  PRO A 372     26.546  54.187  20.457  1.00  0.00      H
ATOM   3266 1HG  PRO A 372     29.583  54.504  20.444  1.00  0.00      H
ATOM   3267 2HG  PRO A 372     28.550  53.872  21.747  1.00  0.00      H
ATOM   3268 1HD  PRO A 372     28.160  51.791  20.597  1.00  0.00      H
ATOM   3269 2HD  PRO A 372     29.796  52.139  19.989  1.00  0.00      H
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ATOM 3270 N LYS A 373 27.735 56.077 17.399 1.00 0.00 N
ATOM 3271 CA LYS A 373 28.261 57.142 16.544 1.00 0.00 C
ATOM 3272 C LYS A 373 29.768 57.381 16.720 1.00 0.00 C
ATOM 3273 O LYS A 373 30.329 57.154 17.795 1.00 0.00 O
ATOM 3274 CB LYS A 373 27.426 58.424 16.694 1.00 0.00 C
ATOM 3275 CG LYS A 373 26.900 58.762 18.102 1.00 0.00 C
ATOM 3276 CD LYS A 373 26.113 60.074 18.000 1.00 0.00 C
ATOM 3277 CE LYS A 373 25.362 60.466 19.281 1.00 0.00 C
ATOM 3278 NZ LYS A 373 24.826 61.842 19.190 1.00 0.00 N1+
ATOM 3279 H LYS A 373 26.856 56.303 17.842 1.00 0.00 H
ATOM 3280 HA LYS A 373 27.961 56.962 15.512 1.00 0.00 H
ATOM 3281 1HB LYS A 373 28.023 59.285 16.392 1.00 0.00 H
ATOM 3282 2HB LYS A 373 26.541 58.358 16.061 1.00 0.00 H
ATOM 3283 1HG LYS A 373 26.253 57.958 18.451 1.00 0.00 H
ATOM 3284 2HG LYS A 373 27.740 58.876 18.787 1.00 0.00 H
ATOM 3285 1HD LYS A 373 26.796 60.892 17.771 1.00 0.00 H
ATOM 3286 2HD LYS A 373 25.368 59.991 17.209 1.00 0.00 H
ATOM 3287 1HE LYS A 373 24.530 59.780 19.439 1.00 0.00 H
ATOM 3288 2HE LYS A 373 26.041 60.414 20.132 1.00 0.00 H
ATOM 3289 1HZ LYS A 373 24.338 62.071 20.044 1.00 0.00 H
ATOM 3290 2HZ LYS A 373 25.587 62.492 19.052 1.00 0.00 H
ATOM 3291 3HZ LYS A 373 24.186 61.903 18.411 1.00 0.00 H
ATOM 3292 N GLY A 374 30.440 57.770 15.637 1.00 0.00 N
ATOM 3293 CA GLY A 374 31.887 57.783 15.532 1.00 0.00 C
ATOM 3294 C GLY A 374 32.440 56.360 15.356 1.00 0.00 C
ATOM 3295 O GLY A 374 33.177 56.059 14.406 1.00 0.00 O
ATOM 3296 H GLY A 374 29.940 58.082 14.817 1.00 0.00 H
ATOM 3297 1HA GLY A 374 32.184 58.382 14.670 1.00 0.00 H
ATOM 3298 2HA GLY A 374 32.314 58.215 16.437 1.00 0.00 H
ATOM 3299 N VAL A 375 32.125 55.466 16.298 1.00 0.00 N
ATOM 3300 CA VAL A 375 32.606 54.098 16.277 1.00 0.00 C
ATOM 3301 C VAL A 375 32.000 53.391 15.061 1.00 0.00 C
ATOM 3302 O VAL A 375 32.741 52.905 14.203 1.00 0.00 O
ATOM 3303 CB VAL A 375 32.357 53.371 17.612 1.00 0.00 C
ATOM 3304 CGI VAL A 375 33.223 52.104 17.669 1.00 0.00 C
ATOM 3305 CG2 VAL A 375 32.705 54.254 18.819 1.00 0.00 C
ATOM 3306 H VAL A 375 31.527 55.732 17.067 1.00 0.00 H
ATOM 3307 HA VAL A 375 33.695 54.095 16.327 1.00 0.00 H
ATOM 3308 HB VAL A 375 31.304 53.099 17.688 1.00 0.00 H
ATOM 3309 1HG1 VAL A 375 33.050 51.587 18.612 1.00 0.00 H
ATOM 3310 2HG1 VAL A 375 32.961 51.447 16.840 1.00 0.00 H
ATOM 3311 3HG1 VAL A 375 34.275 52.380 17.594 1.00 0.00 H
ATOM 3312 1HG2 VAL A 375 32.515 53.702 19.740 1.00 0.00 H
ATOM 3313 2HG2 VAL A 375 33.758 54.533 18.774 1.00 0.00 H
ATOM 3314 3HG2 VAL A 375 32.090 55.153 18.801 1.00 0.00 H
ATOM 3315 N ARG A 376 30.675 53.404 14.931 1.00 0.00 N
ATOM 3316 CA ARG A 376 30.075 53.408 13.608 1.00 0.00 C
ATOM 3317 C ARG A 376 30.325 54.833 13.103 1.00 0.00 C
ATOM 3318 O ARG A 376 29.983 55.779 13.798 1.00 0.00 O
ATOM 3319 CB ARG A 376 28.569 53.050 13.662 1.00 0.00 C
ATOM 3320 CG ARG A 376 27.702 54.251 14.065 1.00 0.00 C
ATOM 3321 CD ARG A 376 26.233 54.021 14.412 1.00 0.00 C
ATOM 3322 NE ARG A 376 25.603 55.330 14.679 1.00 0.00 N
ATOM 3323 CZ ARG A 376 24.654 55.587 15.590 1.00 0.00 C
ATOM 3324 NH1 ARG A 376 24.169 54.624 16.359 1.00 0.00 N1+
ATOM 3325 NH2 ARG A 376 24.172 56.812 15.756 1.00 0.00 N
ATOM 3326 H ARG A 376 30.087 53.410 15.752 1.00 0.00 H
ATOM 3327 HA ARG A 376 30.544 52.639 12.993 1.00 0.00 H
ATOM 3328 1HB ARG A 376 28.240 52.710 12.680 1.00 0.00 H

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ATOM   3329 2HB  ARG A 376     28.410  52.257  14.392  1.00  0.00        H
ATOM   3330 1HG  ARG A 376     28.122  54.721  14.955  1.00  0.00        H
ATOM   3331 2HG  ARG A 376     27.679  54.974  13.250  1.00  0.00        H
ATOM   3332 1HD  ARG A 376     25.734  53.532  13.576  1.00  0.00        H
ATOM   3333 2HD  ARG A 376     26.163  53.388  15.297  1.00  0.00        H
ATOM   3334  HE  ARG A 376     25.954  56.074  14.092  1.00  0.00        H
ATOM   3335 1HH1 ARG A 376     23.454  54.834  17.041  1.00  0.00        H
ATOM   3336 2HH1 ARG A 376     24.514  53.679  16.264  1.00  0.00        H
ATOM   3337 1HH2 ARG A 376     23.457  56.985  16.448  1.00  0.00        H
ATOM   3338 2HH2 ARG A 376     24.521  57.573  15.190  1.00  0.00        H
ATOM   3339  N   HIS A 377     30.919  55.028  11.931  1.00  0.00        N
ATOM   3340  CA  HIS A 377     30.875  56.360  11.348  1.00  0.00        C
ATOM   3341  C   HIS A 377     29.508  56.462  10.672  1.00  0.00        C
ATOM   3342  O   HIS A 377     29.178  55.612   9.839  1.00  0.00        O
ATOM   3343  CB  HIS A 377     32.040  56.568  10.379  1.00  0.00        C
ATOM   3344  CG  HIS A 377     31.862  57.731  9.436  1.00  0.00        C
ATOM   3345  CD2 HIS A 377     32.231  57.902  8.127  1.00  0.00        C
ATOM   3346  ND1 HIS A 377     31.220  58.913  9.787  1.00  0.00        N
ATOM   3347  CE1 HIS A 377     31.127  59.676  8.684  1.00  0.00        C
ATOM   3348  NE2 HIS A 377     31.733  59.097  7.652  1.00  0.00        N
ATOM   3349  H   HIS A 377     31.386  54.262  11.468  1.00  0.00        H
ATOM   3350  HA  HIS A 377     31.033  57.104  12.129  1.00  0.00        H
ATOM   3351 1HB  HIS A 377     32.954  56.751  10.944  1.00  0.00        H
ATOM   3352 2HB  HIS A 377     32.165  55.676   9.765  1.00  0.00        H
ATOM   3353  HD2 HIS A 377     32.827  57.150  7.631  1.00  0.00        H
ATOM   3354  HD1 HIS A 377     30.920  59.061  10.740  1.00  0.00        H
ATOM   3355  HE1 HIS A 377     30.608  60.622   8.724  1.00  0.00        H
ATOM   3356  N   THR A 378     28.722  57.458  11.057  1.00  0.00        N
ATOM   3357  CA  THR A 378     27.334  57.609  10.672  1.00  0.00        C
ATOM   3358  C   THR A 378     27.212  58.680   9.586  1.00  0.00        C
ATOM   3359  O   THR A 378     27.745  59.784   9.720  1.00  0.00        O
ATOM   3360  CB  THR A 378     26.491  57.982  11.904  1.00  0.00        C
ATOM   3361  CG2 THR A 378     25.017  57.653  11.655  1.00  0.00        C
ATOM   3362  OG1 THR A 378     26.930  57.312  13.072  1.00  0.00        O
ATOM   3363  H   THR A 378     29.083  58.182  11.661  1.00  0.00        H
ATOM   3364  HA  THR A 378     26.948  56.652  10.320  1.00  0.00        H
ATOM   3365  HB  THR A 378     26.618  59.042  12.124  1.00  0.00        H
ATOM   3366 1HG2 THR A 378     24.430  57.921  12.534  1.00  0.00        H
ATOM   3367 2HG2 THR A 378     24.658  58.217  10.794  1.00  0.00        H
ATOM   3368 3HG2 THR A 378     24.910  56.586  11.459  1.00  0.00        H
ATOM   3369  HG1 THR A 378     26.380  57.571  13.815  1.00  0.00        H
ATOM   3370  N   MET A 379     26.496  58.357   8.509  1.00  0.00        N
ATOM   3371  CA  MET A 379     26.322  59.222   7.359  1.00  0.00        C
ATOM   3372  C   MET A 379     24.839  59.235   6.998  1.00  0.00        C
ATOM   3373  O   MET A 379     24.299  58.228   6.542  1.00  0.00        O
ATOM   3374  CB  MET A 379     27.147  58.655   6.201  1.00  0.00        C
ATOM   3375  CG  MET A 379     28.654  58.689   6.464  1.00  0.00        C
ATOM   3376  SD  MET A 379     29.600  57.565   5.406  1.00  0.00        S
ATOM   3377  CE  MET A 379     29.529  56.067   6.417  1.00  0.00        C
ATOM   3378  H   MET A 379     26.034  57.461   8.461  1.00  0.00        H
ATOM   3379  HA  MET A 379     26.650  60.231   7.610  1.00  0.00        H
ATOM   3380 1HB  MET A 379     26.865  57.617   6.028  1.00  0.00        H
ATOM   3381 2HB  MET A 379     26.956  59.238   5.299  1.00  0.00        H
ATOM   3382 1HG  MET A 379     29.032  59.697   6.287  1.00  0.00        H
ATOM   3383 2HG  MET A 379     28.850  58.404   7.498  1.00  0.00        H
ATOM   3384 1HE  MET A 379     30.066  55.263   5.914  1.00  0.00        H
ATOM   3385 2HE  MET A 379     29.989  56.260   7.386  1.00  0.00        H
ATOM   3386 3HE  MET A 379     28.489  55.774   6.561  1.00  0.00        H
ATOM   3387  N   MET A 380     24.180  60.373   7.182  1.00  0.00        N
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ATOM 3388 CA MET A 380 22.786 60.549 6.826 1.00 0.00 C
ATOM 3389 C MET A 380 22.740 61.327 5.517 1.00 0.00 C
ATOM 3390 O MET A 380 23.243 62.447 5.452 1.00 0.00 O
ATOM 3391 CB MET A 380 22.072 61.341 7.926 1.00 0.00 C
ATOM 3392 CG MET A 380 21.909 60.537 9.217 1.00 0.00 C
ATOM 3393 SD MET A 380 21.330 61.515 10.631 1.00 0.00 S
ATOM 3394 CE MET A 380 19.605 61.799 10.162 1.00 0.00 C
ATOM 3395 H MET A 380 24.651 61.168 7.589 1.00 0.00 H
ATOM 3396 HA MET A 380 22.318 59.573 6.692 1.00 0.00 H
ATOM 3397 1HB MET A 380 22.646 62.238 8.160 1.00 0.00 H
ATOM 3398 2HB MET A 380 21.078 61.627 7.582 1.00 0.00 H
ATOM 3399 IHG MET A 380 21.183 59.740 9.060 1.00 0.00 H
ATOM 3400 2HG MET A 380 22.869 60.104 9.499 1.00 0.00 H
ATOM 3401 1HE MET A 380 19.110 62.389 10.934 1.00 0.00 H
ATOM 3402 2HE MET A 380 19.569 62.338 9.215 1.00 0.00 H
ATOM 3403 3HE MET A 380 19.094 60.842 10.055 1.00 0.00 H
ATOM 3404 N PHE A 381 22.097 60.758 4.502 1.00 0.00 N
ATOM 3405 CA PHE A 381 21.719 61.462 3.296 1.00 0.00 C
ATOM 3406 C PHE A 381 20.194 61.421 3.226 1.00 0.00 C
ATOM 3407 O PHE A 381 19.572 60.373 3.417 1.00 0.00 O
ATOM 3408 CB PHE A 381 22.337 60.808 2.052 1.00 0.00 C
ATOM 3409 CG PHE A 381 23.849 60.866 1.944 1.00 0.00 C
ATOM 3410 CD1 PHE A 381 24.477 61.822 1.123 1.00 0.00 C
ATOM 3411 CD2 PHE A 381 24.649 59.949 2.650 1.00 0.00 C
ATOM 3412 CE1 PHE A 381 25.877 61.853 0.994 1.00 0.00 C
ATOM 3413 CE2 PHE A 381 26.050 59.985 2.536 1.00 0.00 C
ATOM 3414 CZ PHE A 381 26.667 60.936 1.706 1.00 0.00 C
ATOM 3415 H PHE A 381 21.846 59.780 4.547 1.00 0.00 H
ATOM 3416 HA PHE A 381 22.090 62.485 3.341 1.00 0.00 H
ATOM 3417 1HB PHE A 381 22.075 59.751 2.028 1.00 0.00 H
ATOM 3418 2HB PHE A 381 21.954 61.297 1.156 1.00 0.00 H
ATOM 3419 HD1 PHE A 381 23.883 62.543 0.582 1.00 0.00 H
ATOM 3420 HD2 PHE A 381 24.188 59.209 3.287 1.00 0.00 H
ATOM 3421 HE1 PHE A 381 26.344 62.582 0.348 1.00 0.00 H
ATOM 3422 HE2 PHE A 381 26.654 59.280 3.088 1.00 0.00 H
ATOM 3423 HZ PHE A 381 27.743 60.964 1.614 1.00 0.00 H
ATOM 3424 N SER A 382 19.591 62.561 2.929 1.00 0.00 N
ATOM 3425 CA SER A 382 18.168 62.687 2.705 1.00 0.00 C
ATOM 3426 C SER A 382 18.019 63.660 1.544 1.00 0.00 C
ATOM 3427 O SER A 382 18.862 64.537 1.340 1.00 0.00 O
ATOM 3428 CB SER A 382 17.462 63.176 3.977 1.00 0.00 C
ATOM 3429 OG SER A 382 18.131 64.276 4.570 1.00 0.00 O
ATOM 3430 H SER A 382 20.131 63.411 2.847 1.00 0.00 H
ATOM 3431 HA SER A 382 17.745 61.705 2.497 1.00 0.00 H
ATOM 3432 1HB SER A 382 16.447 63.489 3.731 1.00 0.00 H
ATOM 3433 2HB SER A 382 17.425 62.367 4.707 1.00 0.00 H
ATOM 3434 HG SER A 382 17.659 64.550 5.359 1.00 0.00 H
ATOM 3435 N ALA A 383 16.977 63.497 0.746 1.00 0.00 N
ATOM 3436 CA ALA A 383 16.718 64.414 -0.341 1.00 0.00 C
ATOM 3437 C ALA A 383 16.056 65.694 0.189 1.00 0.00 C
ATOM 3438 O ALA A 383 15.983 66.691 -0.530 1.00 0.00 O
ATOM 3439 CB ALA A 383 15.947 63.664 -1.423 1.00 0.00 C
ATOM 3440 H ALA A 383 16.346 62.722 0.891 1.00 0.00 H
ATOM 3441 HA ALA A 383 17.633 64.567 -0.914 1.00 0.00 H
ATOM 3442 1HB ALA A 383 15.740 64.337 -2.255 1.00 0.00 H
ATOM 3443 2HB ALA A 383 16.542 62.822 -1.777 1.00 0.00 H
ATOM 3444 3HB ALA A 383 15.007 63.296 -1.011 1.00 0.00 H
ATOM 3445 N THR A 384 15.660 65.667 1.462 1.00 0.00 N
ATOM 3446 CA THR A 384 14.938 66.706 2.179 1.00 0.00 C

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ATOM   3447  C   THR A 384     15.766  67.106   3.415  1.00  0.00      C
ATOM   3448  O   THR A 384     16.785  66.469   3.709  1.00  0.00      O
ATOM   3449  CB  THR A 384     13.602  66.087   2.623  1.00  0.00      C
ATOM   3450  CG2 THR A 384     12.809  65.492   1.465  1.00  0.00      C
ATOM   3451  OG1 THR A 384     13.833  65.027   3.529  1.00  0.00      O
ATOM   3452  H   THR A 384     15.857  64.859   2.035  1.00  0.00      H
ATOM   3453  HA  THR A 384     14.828  67.581   1.538  1.00  0.00      H
ATOM   3454  HB  THR A 384     12.973  66.858   3.066  1.00  0.00      H
ATOM   3455 1HG2 THR A 384     11.876  65.070   1.842  1.00  0.00      H
ATOM   3456 2HG2 THR A 384     12.586  66.272   0.737  1.00  0.00      H
ATOM   3457 3HG2 THR A 384     13.395  64.706   0.988  1.00  0.00      H
ATOM   3458  HG1 THR A 384     12.994  64.647   3.799  1.00  0.00      H
ATOM   3459  N   PHE A 385     15.334  68.102   4.190  1.00  0.00      N
ATOM   3460  CA  PHE A 385     15.855  68.358   5.524  1.00  0.00      C
ATOM   3461  C   PHE A 385     14.726  68.811   6.462  1.00  0.00      C
ATOM   3462  O   PHE A 385     14.681  69.972   6.872  1.00  0.00      O
ATOM   3463  CB  PHE A 385     16.986  69.393   5.441  1.00  0.00      C
ATOM   3464  CG  PHE A 385     17.707  69.645   6.753  1.00  0.00      C
ATOM   3465  CD1 PHE A 385     18.547  68.661   7.306  1.00  0.00      C
ATOM   3466  CD2 PHE A 385     17.544  70.864   7.440  1.00  0.00      C
ATOM   3467  CE1 PHE A 385     19.213  68.889   8.523  1.00  0.00      C
ATOM   3468  CE2 PHE A 385     18.218  71.103   8.650  1.00  0.00      C
ATOM   3469  CZ  PHE A 385     19.055  70.114   9.192  1.00  0.00      C
ATOM   3470  H   PHE A 385     14.611  68.723   3.857  1.00  0.00      H
ATOM   3471  HA  PHE A 385     16.362  67.467   5.895  1.00  0.00      H
ATOM   3472 1HB  PHE A 385     17.737  69.054   4.727  1.00  0.00      H
ATOM   3473 2HB  PHE A 385     16.580  70.350   5.114  1.00  0.00      H
ATOM   3474  HD1 PHE A 385     18.686  67.720   6.794  1.00  0.00      H
ATOM   3475  HD2 PHE A 385     16.895  71.628   7.039  1.00  0.00      H
ATOM   3476  HE1 PHE A 385     19.846  68.123   8.944  1.00  0.00      H
ATOM   3477  HE2 PHE A 385     18.091  72.046   9.161  1.00  0.00      H
ATOM   3478  HZ  PHE A 385     19.577  70.293  10.121  1.00  0.00      H
ATOM   3479  N   PRO A 386     13.856  67.886   6.888  1.00  0.00      N
ATOM   3480  CA  PRO A 386     12.648  68.274   7.589  1.00  0.00      C
ATOM   3481  C   PRO A 386     12.948  68.330   9.086  1.00  0.00      C
ATOM   3482  O   PRO A 386     14.035  67.959   9.544  1.00  0.00      O
ATOM   3483  CB  PRO A 386     11.613  67.189   7.266  1.00  0.00      C
ATOM   3484  CG  PRO A 386     12.473  65.962   6.971  1.00  0.00      C
ATOM   3485  CD  PRO A 386     13.642  66.610   6.236  1.00  0.00      C
ATOM   3486  HA  PRO A 386     12.326  69.256   7.243  1.00  0.00      H
ATOM   3487 1HB  PRO A 386     10.960  67.042   8.126  1.00  0.00      H
ATOM   3488 2HB  PRO A 386     11.018  67.498   6.407  1.00  0.00      H
ATOM   3489 1HG  PRO A 386     12.756  65.482   7.907  1.00  0.00      H
ATOM   3490 2HG  PRO A 386     11.907  65.260   6.360  1.00  0.00      H
ATOM   3491 1HD  PRO A 386     13.408  66.774   5.184  1.00  0.00      H
ATOM   3492 2HD  PRO A 386     14.545  66.004   6.316  1.00  0.00      H
ATOM   3493  N   LYS A 387     11.971  68.763   9.886  1.00  0.00      N
ATOM   3494  CA  LYS A 387     12.196  68.920  11.311  1.00  0.00      C
ATOM   3495  C   LYS A 387     12.503  67.568  11.975  1.00  0.00      C
ATOM   3496  O   LYS A 387     13.006  67.541  13.096  1.00  0.00      O
ATOM   3497  CB  LYS A 387     11.053  69.720  11.966  1.00  0.00      C
ATOM   3498  CG  LYS A 387      9.826  68.880  12.358  1.00  0.00      C
ATOM   3499  CD  LYS A 387      9.845  68.463  13.846  1.00  0.00      C
ATOM   3500  CE  LYS A 387      9.678  66.953  14.075  1.00  0.00      C
ATOM   3501  NZ  LYS A 387      8.469  66.391  13.448  1.00  0.00      N1+
ATOM   3502  H   LYS A 387     11.064  68.984   9.501  1.00  0.00      H
ATOM   3503  HA  LYS A 387     12.930  69.709  11.478  1.00  0.00      H
ATOM   3504 1HB  LYS A 387     11.417  70.192  12.879  1.00  0.00      H
ATOM   3505 2HB  LYS A 387     10.703  70.487  11.276  1.00  0.00      H
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ATOM   3506 1HG  LYS A 387      8.919  69.459  12.183  1.00  0.00           H
ATOM   3507 2HG  LYS A 387      9.799  67.973  11.755  1.00  0.00           H
ATOM   3508 1HD  LYS A 387     10.796  68.752  14.294  1.00  0.00           H
ATOM   3509 2HD  LYS A 387      9.030  68.959  14.374  1.00  0.00           H
ATOM   3510 1HE  LYS A 387     10.536  66.425  13.658  1.00  0.00           H
ATOM   3511 2HE  LYS A 387      9.613  66.752  15.145  1.00  0.00           H
ATOM   3512 1HZ  LYS A 387      8.421  65.400  13.637  1.00  0.00           H
ATOM   3513 2HZ  LYS A 387      7.651  66.846  13.828  1.00  0.00           H
ATOM   3514 3HZ  LYS A 387      8.506  66.543  12.450  1.00  0.00           H
ATOM   3515 N    GLU A 388     12.184  66.457  11.300  1.00  0.00           N
ATOM   3516 CA   GLU A 388     12.551  65.116  11.722  1.00  0.00           C
ATOM   3517 C    GLU A 388     14.078  65.006  11.701  1.00  0.00           C
ATOM   3518 O    GLU A 388     14.717  64.791  12.728  1.00  0.00           O
ATOM   3519 CB   GLU A 388     11.924  64.029  10.821  1.00  0.00           C
ATOM   3520 CG   GLU A 388     10.557  64.363  10.209  1.00  0.00           C
ATOM   3521 CD   GLU A 388      9.578  64.881  11.234  1.00  0.00           C
ATOM   3522 OE1  GLU A 388      9.509  64.317  12.348  1.00  0.00           O
ATOM   3523 OE2  GLU A 388      8.955  65.931  10.972  1.00  0.00           Ol-
ATOM   3524 H    GLU A 388     11.656  66.522  10.441  1.00  0.00           H
ATOM   3525 HA   GLU A 388     12.149  64.924  12.717  1.00  0.00           H
ATOM   3526 1HB  GLU A 388     12.587  63.825   9.981  1.00  0.00           H
ATOM   3527 2HB  GLU A 388     11.779  63.116  11.399  1.00  0.00           H
ATOM   3528 1HG  GLU A 388     10.678  65.129   9.443  1.00  0.00           H
ATOM   3529 2HG  GLU A 388     10.130  63.465   9.761  1.00  0.00           H
ATOM   3530 N    ILE A 389     14.668  65.151  10.513  1.00  0.00           N
ATOM   3531 CA   ILE A 389     16.100  65.020  10.300  1.00  0.00           C
ATOM   3532 C    ILE A 389     16.826  66.077  11.137  1.00  0.00           C
ATOM   3533 O    ILE A 389     17.913  65.836  11.663  1.00  0.00           O
ATOM   3534 CB   ILE A 389     16.414  65.150   8.795  1.00  0.00           C
ATOM   3535 CGI  ILE A 389     15.814  64.004   7.954  1.00  0.00           C
ATOM   3536 CG2  ILE A 389     17.920  65.248   8.535  1.00  0.00           C
ATOM   3537 CD1  ILE A 389     16.494  62.643   8.143  1.00  0.00           C
ATOM   3538 H    ILE A 389     14.113  65.363   9.696  1.00  0.00           H
ATOM   3539 HA   ILE A 389     16.414  64.007  10.551  1.00  0.00           H
ATOM   3540 HB   ILE A 389     16.073  66.121   8.434  1.00  0.00           H
ATOM   3541 1HG1 ILE A 389     14.765  63.870   8.219  1.00  0.00           H
ATOM   3542 2HG1 ILE A 389     15.892  64.250   6.895  1.00  0.00           H
ATOM   3543 1HG2 ILE A 389     18.100  65.338   7.463  1.00  0.00           H
ATOM   3544 2HG2 ILE A 389     18.321  66.124   9.045  1.00  0.00           H
ATOM   3545 3HG2 ILE A 389     18.414  64.352   8.911  1.00  0.00           H
ATOM   3546 1HD1 ILE A 389     16.004  61.901   7.513  1.00  0.00           H
ATOM   3547 2HD1 ILE A 389     17.545  62.719   7.864  1.00  0.00           H
ATOM   3548 3HD1 ILE A 389     16.417  62.340   9.187  1.00  0.00           H
ATOM   3549 N    GLN A 390     16.225  67.259  11.256  1.00  0.00           N
ATOM   3550 CA   GLN A 390     16.803  68.366  11.989  1.00  0.00           C
ATOM   3551 C    GLN A 390     16.964  68.025  13.479  1.00  0.00           C
ATOM   3552 O    GLN A 390     17.757  68.667  14.175  1.00  0.00           O
ATOM   3553 CB   GLN A 390     15.929  69.603  11.771  1.00  0.00           C
ATOM   3554 CG   GLN A 390     16.664  70.917  12.044  1.00  0.00           C
ATOM   3555 CD   GLN A 390     15.806  72.113  11.654  1.00  0.00           C
ATOM   3556 NE2  GLN A 390     15.407  72.207  10.392  1.00  0.00           N
ATOM   3557 OE1  GLN A 390     15.503  72.956  12.490  1.00  0.00           O
ATOM   3558 H    GLN A 390     15.324  67.414  10.825  1.00  0.00           H
ATOM   3559 HA   GLN A 390     17.754  68.645  11.536  1.00  0.00           H
ATOM   3560 1HB  GLN A 390     15.585  69.628  10.737  1.00  0.00           H
ATOM   3561 2HB  GLN A 390     15.068  69.563  12.439  1.00  0.00           H
ATOM   3562 1HG  GLN A 390     16.901  70.988  13.105  1.00  0.00           H
ATOM   3563 2HG  GLN A 390     17.586  70.945  11.464  1.00  0.00           H
ATOM   3564 1HE2 GLN A 390     14.837  72.987  10.099  1.00  0.00           H
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ATOM 3565 2HE2 GLN A 390 15.673 71.497 9.724 1.00 0.00 H
ATOM 3566 N MET A 391 16.217 67.032 13.966 1.00 0.00 N
ATOM 3567 CA MET A 391 16.3 15 66.505 15.3 16 1.00 0.00 C
ATOM 3568 C MET A 391 17.173 65.243 15.287 1.00 0.00 C
ATOM 3569 O MET A 391 18.144 65.148 16.027 1.00 0.00 O
ATOM 3570 CB MET A 391 14.919 66.213 15.881 1.00 0.00 C
ATOM 3571 CG MET A 391 14.157 67.5 11 16.167 1.00 0.00 C
ATOM 3572 SD MET A 391 12.416 67.299 16.634 1.00 0.00 S
ATOM 3573 CE MET A 391 12.585 66.3 11 18.144 1.00 0.00 C
ATOM 3574 H MET A 391 15.522 66.589 13.382 1.00 0.00 H
ATOM 3575 HA MET A 391 16.738 67.264 15.973 1.00 0.00 H
ATOM 3576 1HB MET A 391 14.350 65.627 15.159 1.00 0.00 H
ATOM 3577 2HB MET A 391 15.013 65.652 16.810 1.00 0.00 H
ATOM 3578 1HG MET A 391 14.635 68.040 16.991 1.00 0.00 H
ATOM 3579 2HG MET A 391 14.164 68. 141 15.278 1.00 0.00 H
ATOM 3580 1HE MET A 391 11.597 66.098 18.552 1.00 0.00 H
ATOM 3581 2HE MET A 391 13.091 65.375 17.91 1 1.00 0.00 H
ATOM 3582 3HE MET A 391 13.169 66.866 18.878 1.00 0.00 H
ATOM 3583 N LEU A 392 16.840 64.290 14.420 1.00 0.00 N
ATOM 3584 CA LEU A 392 17.452 62.966 14.391 1.00 0.00 C
ATOM 3585 C LEU A 392 18.960 63.057 14. 109 1.00 0.00 C
ATOM 3586 O LEU A 392 19.726 62.139 14.396 1.00 0.00 O
ATOM 3587 CB LEU A 392 16.717 62. 135 13.328 1.00 0.00 C
ATOM 3588 CG LEU A 392 16.990 60.623 13.355 1.00 0.00 C
ATOM 3589 CD1 LEU A 392 16.45 1 59.978 14.635 1.00 0.00 C
ATOM 3590 CD2 LEU A 392 16.282 59.989 12.152 1.00 0.00 C
ATOM 3591 H LEU A 392 16.125 64.463 13.729 1.00 0.00 H
ATOM 3592 HA LEU A 392 17.261 62.456 15.335 1.00 0.00 H
ATOM 3593 1HB LEU A 392 15.641 62.252 13.454 1.00 0.00 H
ATOM 3594 2HB LEU A 392 17.006 62.478 12.334 1.00 0.00 H
ATOM 3595 HG LEU A 392 18.065 60.447 13.3 17 1.00 0.00 H
ATOM 3596 1HD1 LEU A 392 16.661 58.909 14.620 1.00 0.00 H
ATOM 3597 2HD1 LEU A 392 16.933 60.43 1 15.501 1.00 0.00 H
ATOM 3598 3HD1 LEU A 392 15.374 60. 136 14.696 1.00 0.00 H
ATOM 3599 1HD2 LEU A 392 16.462 58.914 12. 149 1.00 0.00 H
ATOM 3600 2HD2 LEU A 392 15.21 1 60.178 12.21 8 1.00 0.00 H
ATOM 3601 3HD2 LEU A 392 16.671 60.424 11.230 1.00 0.00 H
ATOM 3602 N ALA A 393 19.409 64. 179 13.544 1.00 0.00 N
ATOM 3603 CA ALA A 393 20.817 64.449 13.3 15 1.00 0.00 C
ATOM 3604 C ALA A 393 2 1.501 64.980 14.586 1.00 0.00 C
ATOM 3605 O ALA A 393 22.583 65.568 14.510 1.00 0.00 O
ATOM 3606 CB ALA A 393 20.946 65.436 12.149 1.00 0.00 C
ATOM 3607 H ALA A 393 18.758 64.893 13.252 1.00 0.00 H
ATOM 3608 HA ALA A 393 2 1.306 63.546 12.950 1.00 0.00 H
ATOM 3609 1HB ALA A 393 2 1.999 65.647 11.966 1.00 0.00 H
ATOM 3610 2HB ALA A 393 20.503 65.000 11.254 1.00 0.00 H
ATOM 361 1 3HB ALA A 393 20.428 66.362 12.397 1.00 0.00 H
ATOM 3612 N ARG A 394 20.858 64.875 15.752 1.00 0.00 N
ATOM 3613 CA ARG A 394 2 1.453 65.023 17.076 1.00 0.00 C
ATOM 3614 C ARG A 394 2 1.645 63.61 1 17.626 1.00 0.00 C
ATOM 3615 O ARG A 394 22.71 1 63.278 18. 143 1.00 0.00 O
ATOM 3616 CB ARG A 394 20.543 65.814 18.038 1.00 0.00 C
ATOM 3617 CG ARG A 394 20.532 67.350 17.926 1.00 0.00 C
ATOM 361 8 CD ARG A 394 20.071 67.924 16.580 1.00 0.00 C
ATOM 3619 NE ARG A 394 2 1.122 67.766 15.572 1.00 0.00 N
ATOM 3620 CZ ARG A 394 21.256 68.432 14.426 1.00 0.00 C
ATOM 3621 NH1 ARG A 394 20.349 69.329 14.046 1.00 0.00 N1+
ATOM 3622 NH2 ARG A 394 22.323 68. 169 13.682 1.00 0.00 N
ATOM 3623 H ARG A 394 19.868 64.677 15.766 1.00 0.00 H

ATOM 3624 HA ARG A 394 22.416 65.525 16.988 1.00 0.00 H
ATOM 3625 1HB ARG A 394 19.506 65.513 17.889 1.00 0.00 H
ATOM 3626 2HB ARG A 394 20.836 65.608 19.068 1.00 0.00 H
ATOM 3627 1HG ARG A 394 19.860 67.765 18.678 1.00 0.00 H
ATOM 3628 2HG ARG A 394 21.539 67.734 18.088 1.00 0.00 H
ATOM 3629 1HD ARG A 394 19.177 67.396 16.247 1.00 0.00 H
ATOM 3630 2HD ARG A 394 19.845 68.984 16.695 1.00 0.00 H
ATOM 3631 HE ARG A 394 21.795 67.057 15.826 1.00 0.00 H
ATOM 3632 1HH1 ARG A 394 20.465 69.826 13.174 1.00 0.00 H
ATOM 3633 2HH1 ARG A 394 19.545 69.512 14.629 1.00 0.00 H
ATOM 3634 1HH2 ARG A 394 22.460 68.653 12.806 1.00 0.00 H
ATOM 3635 2HH2 ARG A 394 22.997 67.484 13.991 1.00 0.00 H
ATOM 3636 N ASP A 395 20.602 62.789 17.527 1.00 0.00 N
ATOM 3637 CA ASP A 395 20.645 61.390 17.897 1.00 0.00 C
ATOM 3638 C ASP A 395 21.814 60.736 17.172 1.00 0.00 C
ATOM 3639 O ASP A 395 22.777 60.280 17.786 1.00 0.00 O
ATOM 3640 CB ASP A 395 19.349 60.673 17.499 1.00 0.00 C
ATOM 3641 CG ASP A 395 18.129 61.176 18.237 1.00 0.00 C
ATOM 3642 OD1 ASP A 395 17.856 62.388 18.130 1.00 0.00 O
ATOM 3643 OD2 ASP A 395 17.456 60.321 18.854 1.00 0.00 Ol-
ATOM 3644 H ASP A 395 19.718 63.134 17.179 1.00 0.00 H
ATOM 3645 HA ASP A 395 20.785 61.302 18.974 1.00 0.00 H
ATOM 3646 1HB ASP A 395 19.166 60.814 16.434 1.00 0.00 H
ATOM 3647 2HB ASP A 395 19.442 59.608 17.713 1.00 0.00 H
ATOM 3648 N PHE A 396 21.712 60.665 15.847 1.00 0.00 N
ATOM 3649 CA PHE A 396 22.493 59.724 15.076 1.00 0.00 C
ATOM 3650 C PHE A 396 23.944 60.156 14.903 1.00 0.00 C
ATOM 3651 O PHE A 396 24.763 59.303 14.564 1.00 0.00 O
ATOM 3652 CB PHE A 396 21.840 59.492 13.707 1.00 0.00 C
ATOM 3653 CG PHE A 396 20.611 58.602 13.660 1.00 0.00 C
ATOM 3654 CD1 PHE A 396 20.070 57.999 14.815 1.00 0.00 C
ATOM 3655 CD2 PHE A 396 19.987 58.360 12.420 1.00 0.00 C
ATOM 3656 CE1 PHE A 396 18.934 57.184 14.726 1.00 0.00 C
ATOM 3657 CE2 PHE A 396 18.840 57.551 12.333 1.00 0.00 C
ATOM 3658 CZ PHE A 396 18.305 56.968 13.492 1.00 0.00 C
ATOM 3659 H PHE A 396 21.076 61.278 15.356 1.00 0.00 H
ATOM 3660 HA PHE A 396 22.438 58.739 15.539 1.00 0.00 H
ATOM 3661 1HB PHE A 396 21.521 60.447 13.290 1.00 0.00 H
ATOM 3662 2HB PHE A 396 22.560 59.024 13.035 1.00 0.00 H
ATOM 3663 HD1 PHE A 396 20.532 58.163 15.777 1.00 0.00 H
ATOM 3664 HD2 PHE A 396 20.389 58.798 11.518 1.00 0.00 H
ATOM 3665 HE1 PHE A 396 18.535 56.716 15.613 1.00 0.00 H
ATOM 3666 HE2 PHE A 396 18.371 57.380 11.375 1.00 0.00 H
ATOM 3667 HZ PHE A 396 17.417 56.357 13.439 1.00 0.00 H
ATOM 3668 N LEU A 397 24.257 61.436 15.106 1.00 0.00 N
ATOM 3669 CA LEU A 397 25.547 62.032 14.763 1.00 0.00 C
ATOM 3670 C LEU A 397 26.107 62.747 15.994 1.00 0.00 C
ATOM 3671 O LEU A 397 25.330 63.184 16.841 1.00 0.00 O
ATOM 3672 CB LEU A 397 25.373 63.074 13.643 1.00 0.00 C
ATOM 3673 CG LEU A 397 24.502 62.659 12.446 1.00 0.00 C
ATOM 3674 CD1 LEU A 397 24.434 63.823 11.456 1.00 0.00 C
ATOM 3675 CD2 LEU A 397 25.042 61.438 11.700 1.00 0.00 C
ATOM 3676 H LEU A 397 23.582 62.061 15.522 1.00 0.00 H
ATOM 3677 HA LEU A 397 26.245 61.248 14.471 1.00 0.00 H
ATOM 3678 1HB LEU A 397 24.909 63.972 14.050 1.00 0.00 H
ATOM 3679 2HB LEU A 397 26.348 63.327 13.227 1.00 0.00 H
ATOM 3680 HG LEU A 397 23.499 62.412 12.794 1.00 0.00 H
ATOM 3681 1HD1 LEU A 397 23.819 63.539 10.602 1.00 0.00 H
ATOM 3682 2HD1 LEU A 397 23.997 64.693 11.946 1.00 0.00 H

ATOM 3683 3HD1 LEU A 397 25.440 64.067 11.113 1.00 0.00 H
ATOM 3684 1HD2 LEU A 397 24.381 61.198 10.867 1.00 0.00 H
ATOM 3685 2HD2 LEU A 397 26.040 61.657 11.320 1.00 0.00 H
ATOM 3686 3HD2 LEU A 397 25.092 60.588 12.381 1.00 0.00 H
ATOM 3687 N ASP A 398 27.429 62.899 16.076 1.00 0.00 N
ATOM 3688 CA ASP A 398 28.127 63.704 17.079 1.00 0.00 C
ATOM 3689 C ASP A 398 29.249 64.429 16.347 1.00 0.00 C
ATOM 3690 O ASP A 398 29.676 63.957 15.294 1.00 0.00 O
ATOM 3691 CB ASP A 398 28.770 62.845 18.186 1.00 0.00 C
ATOM 3692 CG ASP A 398 27.887 62.604 19.395 1.00 0.00 C
ATOM 3693 OD1 ASP A 398 26.929 63.380 19.600 1.00 0.00 O
ATOM 3694 OD2 ASP A 398 28.123 61.590 20.079 1.00 0.00 Ol-
ATOM 3695 H ASP A 398 28.033 62.439 15.410 1.00 0.00 H
ATOM 3696 HA ASP A 398 27.441 64.440 17.497 1.00 0.00 H
ATOM 3697 1HB ASP A 398 29.026 61.865 17.784 1.00 0.00 H
ATOM 3698 2HB ASP A 398 29.673 63.335 18.549 1.00 0.00 H
ATOM 3699 N GLU A 399 29.712 65.545 16.925 1.00 0.00 N
ATOM 3700 CA GLU A 399 30.709 66.476 16.400 1.00 0.00 C
ATOM 3701 C GLU A 399 30.763 66.408 14.866 1.00 0.00 C
ATOM 3702 O GLU A 399 31.700 65.867 14.275 1.00 0.00 O
ATOM 3703 CB GLU A 399 32.064 66.231 17.096 1.00 0.00 C
ATOM 3704 CG GLU A 399 32.846 67.529 17.353 1.00 0.00 C
ATOM 3705 CD GLU A 399 33.160 68.267 16.067 1.00 0.00 C
ATOM 3706 OE1 GLU A 399 32.206 68.755 15.428 1.00 0.00 O
ATOM 3707 OE2 GLU A 399 34.346 68.324 15.687 1.00 0.00 Ol-
ATOM 3708 H GLU A 399 29.366 65.825 17.832 1.00 0.00 H
ATOM 3709 HA GLU A 399 30.524 67.472 16.802 1.00 0.00 H
ATOM 3710 1HB GLU A 399 31.896 65.748 18.059 1.00 0.00 H
ATOM 3711 2HB GLU A 399 32.683 65.588 16.471 1.00 0.00 H
ATOM 3712 1HG GLU A 399 32.256 68.190 17.989 1.00 0.00 H
ATOM 3713 2HG GLU A 399 33.788 67.295 17.849 1.00 0.00 H
ATOM 3714 N TYR A 400 29.721 66.938 14.229 1.00 0.00 N
ATOM 3715 CA TYR A 400 29.309 66.470 12.920 1.00 0.00 C
ATOM 3716 C TYR A 400 29.487 67.571 11.875 1.00 0.00 C
ATOM 3717 O TYR A 400 29.532 68.758 12.211 1.00 0.00 O
ATOM 3718 CB TYR A 400 27.854 65.969 13.001 1.00 0.00 C
ATOM 3719 CG TYR A 400 26.773 66.994 12.705 1.00 0.00 C
ATOM 3720 CD1 TYR A 400 26.089 66.956 11.477 1.00 0.00 C
ATOM 3721 CD2 TYR A 400 26.433 67.995 13.634 1.00 0.00 C
ATOM 3722 CE1 TYR A 400 25.091 67.895 11.182 1.00 0.00 C
ATOM 3723 CE2 TYR A 400 25.436 68.941 13.335 1.00 0.00 C
ATOM 3724 CZ TYR A 400 24.752 68.898 12.105 1.00 0.00 C
ATOM 3725 OH TYR A 400 23.768 69.804 11.812 1.00 0.00 O
ATOM 3726 H TYR A 400 29.195 67.687 14.656 1.00 0.00 H
ATOM 3727 HA TYR A 400 29.866 65.568 12.664 1.00 0.00 H
ATOM 3728 1HB TYR A 400 27.706 65.162 12.285 1.00 0.00 H
ATOM 3729 2HB TYR A 400 27.651 65.603 14.008 1.00 0.00 H
ATOM 3730 HD1 TYR A 400 26.330 66.197 10.748 1.00 0.00 H
ATOM 3731 HD2 TYR A 400 26.939 68.042 14.587 1.00 0.00 H
ATOM 3732 HE1 TYR A 400 24.573 67.853 10.235 1.00 0.00 H
ATOM 3733 HE2 TYR A 400 25.188 69.710 14.052 1.00 0.00 H
ATOM 3734 HH TYR A 400 23.665 70.414 12.546 1.00 0.00 H
ATOM 3735 N ILE A 401 29.548 67.186 10.602 1.00 0.00 N
ATOM 3736 CA ILE A 401 29.545 68.129 9.496 1.00 0.00 C
ATOM 3737 C ILE A 401 28.161 68.090 8.856 1.00 0.00 C
ATOM 3738 O ILE A 401 27.599 67.014 8.652 1.00 0.00 O
ATOM 3739 CB ILE A 401 30.644 67.795 8.472 1.00 0.00 C
ATOM 3740 CG1 ILE A 401 32.046 67.691 9.099 1.00 0.00 C
ATOM 3741 CG2 ILE A 401 30.645 68.842 7.345 1.00 0.00 C

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ATOM   3742  CD1 ILE A 401      32.524  68.980   9.774  1.00  0.00           C
ATOM   3743  H   ILE A 401      29.598  66.203  10.373  1.00  0.00           H
ATOM   3744  HA  ILE A 401      29.802  69.122   9.864  1.00  0.00           H
ATOM   3745  HB  ILE A 401      30.391  66.869   7.955  1.00  0.00           H
ATOM   3746 1HG1 ILE A 401      32.048  66.910   9.860  1.00  0.00           H
ATOM   3747 2HG1 ILE A 401      32.774  67.444   8.325  1.00  0.00           H
ATOM   3748 1HG2 ILE A 401      31.425  68.600   6.624  1.00  0.00           H
ATOM   3749 2HG2 ILE A 401      29.676  68.841   6.846  1.00  0.00           H
ATOM   3750 3HG2 ILE A 401      30.834  69.830   7.767  1.00  0.00           H
ATOM   3751 1HD1 ILE A 401      33.519  68.825  10.191  1.00  0.00           H
ATOM   3752 2HD1 ILE A 401      32.560  69.784   9.038  1.00  0.00           H
ATOM   3753 3HD1 ILE A 401      31.834  69.250  10.573  1.00  0.00           H
ATOM   3754  N   PHE A 402      27.626  69.263   8.522  1.00  0.00           N
ATOM   3755  CA  PHE A 402      26.339  69.407   7.880  1.00  0.00           C
ATOM   3756  C   PHE A 402      26.573  69.949   6.477  1.00  0.00           C
ATOM   3757  O   PHE A 402      27.143  71.025   6.323  1.00  0.00           O
ATOM   3758  CB  PHE A 402      25.487  70.399   8.679  1.00  0.00           C
ATOM   3759  CG  PHE A 402      24.065  70.617   8.193  1.00  0.00           C
ATOM   3760  CD1 PHE A 402      23.399  69.689   7.360  1.00  0.00           C
ATOM   3761  CD2 PHE A 402      23.388  71.795   8.565  1.00  0.00           C
ATOM   3762  CE1 PHE A 402      22.104  69.951   6.887  1.00  0.00           C
ATOM   3763  CE2 PHE A 402      22.092  72.057   8.092  1.00  0.00           C
ATOM   3764  CZ  PHE A 402      21.454  71.139   7.246  1.00  0.00           C
ATOM   3765  H   PHE A 402      28.126  70.119   8.716  1.00  0.00           H
ATOM   3766  HA  PHE A 402      25.853  68.433   7.816  1.00  0.00           H
ATOM   3767 1HB  PHE A 402      25.400  70.057   9.710  1.00  0.00           H
ATOM   3768 2HB  PHE A 402      25.961  71.381   8.661  1.00  0.00           H
ATOM   3769  HD1 PHE A 402      23.887  68.767   7.080  1.00  0.00           H
ATOM   3770  HD2 PHE A 402      23.866  72.508   9.220  1.00  0.00           H
ATOM   3771  HE1 PHE A 402      21.608  69.235   6.248  1.00  0.00           H
ATOM   3772  HE2 PHE A 402      21.585  72.966   8.381  1.00  0.00           H
ATOM   3773  HZ  PHE A 402      20.464  71.348   6.870  1.00  0.00           H
ATOM   3774  N   LEU A 403      26.107  69.231   5.465  1.00  0.00           N
ATOM   3775  CA  LEU A 403      26.089  69.676   4.090  1.00  0.00           C
ATOM   3776  C   LEU A 403      24.646  69.585   3.609  1.00  0.00           C
ATOM   3777  O   LEU A 403      23.930  68.651   3.975  1.00  0.00           O
ATOM   3778  CB  LEU A 403      27.063  68.815   3.272  1.00  0.00           C
ATOM   3779  CG  LEU A 403      27.109  69.164   1.773  1.00  0.00           C
ATOM   3780  CD1 LEU A 403      28.512  68.870   1.226  1.00  0.00           C
ATOM   3781  CD2 LEU A 403      26.094  68.350   0.956  1.00  0.00           C
ATOM   3782  H   LEU A 403      25.732  68.308   5.631  1.00  0.00           H
ATOM   3783  HA  LEU A 403      26.501  70.684   4.029  1.00  0.00           H
ATOM   3784 1HB  LEU A 403      28.074  68.940   3.661  1.00  0.00           H
ATOM   3785 2HB  LEU A 403      26.773  67.767   3.347  1.00  0.00           H
ATOM   3786  HG  LEU A 403      26.879  70.221   1.638  1.00  0.00           H
ATOM   3787 1HD1 LEU A 403      28.548  69.116   0.165  1.00  0.00           H
ATOM   3788 2HD1 LEU A 403      29.246  69.471   1.764  1.00  0.00           H
ATOM   3789 3HD1 LEU A 403      28.740  67.812   1.361  1.00  0.00           H
ATOM   3790 1HD2 LEU A 403      26.163  68.631  -0.095  1.00  0.00           H
ATOM   3791 2HD2 LEU A 403      26.310  67.287   1.062  1.00  0.00           H
ATOM   3792 3HD2 LEU A 403      25.087  68.554   1.320  1.00  0.00           H
ATOM   3793  N   ALA A 404      24.219  70.531   2.777  1.00  0.00           N
ATOM   3794  CA  ALA A 404      22.895  70.506   2.193  1.00  0.00           C
ATOM   3795  C   ALA A 404      22.923  71.159   0.818  1.00  0.00           C
ATOM   3796  O   ALA A 404      23.498  72.234   0.665  1.00  0.00           O
ATOM   3797  CB  ALA A 404      21.910  71.254   3.083  1.00  0.00           C
ATOM   3798  H   ALA A 404      24.826  71.301   2.534  1.00  0.00           H
ATOM   3799  HA  ALA A 404      22.558  69.474   2.100  1.00  0.00           H
ATOM   3800 1HB  ALA A 404      20.918  71.227   2.631  1.00  0.00           H
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ATOM   3801 2HB  ALA A 404      21.874  70.781   4.064  1.00  0.00           H
ATOM   3802 3HB  ALA A 404      22.231  72.290   3.191  1.00  0.00           H
ATOM   3803  N   VAL A 405      22.256  70.539  -0.152  1.00  0.00           N
ATOM   3804  CA  VAL A 405      21.759  71.169  -1.365  1.00  0.00           C
ATOM   3805  C   VAL A 405      20.328  70.646  -1.543  1.00  0.00           C
ATOM   3806  O   VAL A 405      19.987  69.959  -2.508  1.00  0.00           O
ATOM   3807  CB  VAL A 405      22.695  70.912  -2.566  1.00  0.00           C
ATOM   3808  CGI VAL A 405      23.991  71.722  -2.422  1.00  0.00           C
ATOM   3809  CG2 VAL A 405      23.071  69.437  -2.770  1.00  0.00           C
ATOM   3810  H   VAL A 405      22.059  69.551  -0.077  1.00  0.00           H
ATOM   3811  HA  VAL A 405      21.861  72.251  -1.281  1.00  0.00           H
ATOM   3812  HB  VAL A 405      22.179  71.168  -3.491  1.00  0.00           H
ATOM   3813 1HG1 VAL A 405      24.638  71.528  -3.277  1.00  0.00           H
ATOM   3814 2HG1 VAL A 405      23.753  72.785  -2.380  1.00  0.00           H
ATOM   3815 3HG1 VAL A 405      24.503  71.429  -1.506  1.00  0.00           H
ATOM   3816 1HG2 VAL A 405      23.730  69.345  -3.633  1.00  0.00           H
ATOM   3817 2HG2 VAL A 405      23.583  69.066  -1.882  1.00  0.00           H
ATOM   3818 3HG2 VAL A 405      22.167  68.851  -2.939  1.00  0.00           H
ATOM   3819  N   GLY A 406      19.507  70.933  -0.536  1.00  0.00           N
ATOM   3820  CA  GLY A 406      18.150  70.439  -0.371  1.00  0.00           C
ATOM   3821  C   GLY A 406      17.650  70.826   1.023  1.00  0.00           C
ATOM   3822  O   GLY A 406      18.354  71.525   1.752  1.00  0.00           O
ATOM   3823  H   GLY A 406      19.813  71.548   0.205  1.00  0.00           H
ATOM   3824 1HA  GLY A 406      17.506  70.884  -1.130  1.00  0.00           H
ATOM   3825 2HA  GLY A 406      18.142  69.355  -0.478  1.00  0.00           H
ATOM   3826 HXT  GLY A 406      16.684  70.487   1.368  1.00  0.00           H
ATOM   3827  N   THR A 411      16.873  68.679  -11.615  1.00  0.00          N1+
ATOM   3828  CA  THR A 411      18.079  68.144  -10.968  1.00  0.00           C
ATOM   3829  C   THR A 411      18.867  69.321  -10.420  1.00  0.00           C
ATOM   3830  O   THR A 411      18.663  70.441  -10.878  1.00  0.00           O
ATOM   3831  CB  THR A 411      18.916  67.332  -11.957  1.00  0.00           C
ATOM   3832 1H   THR A 411      16.326  67.918  -11.991  1.00  0.00           H
ATOM   3833 2H   THR A 411      16.323  69.185  -10.935  1.00  0.00           H
ATOM   3834 3H   THR A 411      17.140  69.303  -12.363  1.00  0.00           H
ATOM   3835  HA  THR A 411      17.791  67.446  -10.182  1.00  0.00           H
ATOM   3836 1HB  THR A 411      19.802  66.947  -11.453  1.00  0.00           H
ATOM   3837 2HB  THR A 411      18.324  66.499  -12.336  1.00  0.00           H
ATOM   3838 3HB  THR A 411      19.219  67.970  -12.787  1.00  0.00           H
ATOM   3839  N   SER A 412      19.767  69.086   -9.471  1.00  0.00           N
ATOM   3840  CA  SER A 412      20.538  70.113   -8.792  1.00  0.00           C
ATOM   3841  C   SER A 412      21.360  70.960   -9.774  1.00  0.00           C
ATOM   3842  O   SER A 412      21.857  72.024   -9.414  1.00  0.00           O
ATOM   3843  CB  SER A 412      21.427  69.422   -7.742  1.00  0.00           C
ATOM   3844  OG  SER A 412      21.420  68.004   -7.897  1.00  0.00           O
ATOM   3845  H   SER A 412      19.954  68.138   -9.177  1.00  0.00           H
ATOM   3846  HA  SER A 412      19.870  70.737   -8.199  1.00  0.00           H
ATOM   3847 1HB  SER A 412      22.454  69.773   -7.845  1.00  0.00           H
ATOM   3848 2HB  SER A 412      21.061  69.659   -6.743  1.00  0.00           H
ATOM   3849  HG  SER A 412      21.983  67.606   -7.228  1.00  0.00           H
ATOM   3850  N   GLU A 413      21.539  70.456  -10.992  1.00  0.00           N
ATOM   3851  CA  GLU A 413      22.403  71.002  -12.008  1.00  0.00           C
ATOM   3852  C   GLU A 413      21.575  71.603  -13.156  1.00  0.00           C
ATOM   3853  O   GLU A 413      22.149  72.061  -14.141  1.00  0.00           O
ATOM   3854  CB  GLU A 413      23.292  69.859  -12.538  1.00  0.00           C
ATOM   3855  CG  GLU A 413      23.922  68.967  -11.443  1.00  0.00           C
ATOM   3856  CD  GLU A 413      22.963  67.960  -10.816  1.00  0.00           C
ATOM   3857  OE1 GLU A 413      23.309  67.416   -9.747  1.00  0.00           O
ATOM   3858  OE2 GLU A 413      21.864  67.764  -11.374  1.00  0.00          O1-
ATOM   3859  H   GLU A 413      21.045  69.619  -11.270  1.00  0.00           H
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ATOM 3860 HA GLU A 413 23.031 71.779 -11.572 1.00 0.00 H
ATOM 3861 1HB GLU A 413 22.699 69.203 -13.175 1.00 0.00 H
ATOM 3862 2HB GLU A 413 24.116 70.277 -13.115 1.00 0.00 H
ATOM 3863 1HG GLU A 413 24.746 68.395 -11.869 1.00 0.00 H
ATOM 3864 2HG GLU A 413 24.295 69.594 -10.633 1.00 0.00 H
ATOM 3865 N ASN A 414 20.239 71.504 -13.105 1.00 0.00 N
ATOM 3866 CA ASN A 414 19.373 71.780 -14.254 1.00 0.00 C
ATOM 3867 C ASN A 414 17.903 71.584 -13.863 1.00 0.00 C
ATOM 3868 O ASN A 414 17.521 70.472 -13.493 1.00 0.00 O
ATOM 3869 CB ASN A 414 19.757 70.812 -15.383 1.00 0.00 C
ATOM 3870 CG ASN A 414 18.696 70.619 -16.458 1.00 0.00 C
ATOM 3871 ND2 ASN A 414 18.745 69.469 -17.110 1.00 0.00 N
ATOM 3872 OD1 ASN A 414 17.852 71.466 -16.726 1.00 0.00 O
ATOM 3873 H ASN A 414 19.785 71.227 -12.247 1.00 0.00 H
ATOM 3874 HA ASN A 414 19.527 72.806 -14.588 1.00 0.00 H
ATOM 3875 1HB ASN A 414 20.649 71.180 -15.890 1.00 0.00 H
ATOM 3876 2HB ASN A 414 19.958 69.826 -14.964 1.00 0.00 H
ATOM 3877 1HD2 ASN A 414 18.072 69.271 -17.837 1.00 0.00 H
ATOM 3878 2HD2 ASN A 414 19.455 68.788 -16.881 1.00 0.00 H
ATOM 3879 N ILE A 415 17.078 72.631 -13.959 1.00 0.00 N
ATOM 3880 CA ILE A 415 15.694 72.657 -13.494 1.00 0.00 C
ATOM 3881 C ILE A 415 14.880 73.536 -14.453 1.00 0.00 C
ATOM 3882 O ILE A 415 15.342 74.613 -14.829 1.00 0.00 O
ATOM 3883 CB ILE A 415 15.634 73.253 -12.067 1.00 0.00 C
ATOM 3884 CGI ILE A 415 16.562 72.516 -11.087 1.00 0.00 C
ATOM 3885 CG2 ILE A 415 14.196 73.214 -11.540 1.00 0.00 C
ATOM 3886 CD1 ILE A 415 16.486 73.017 -9.641 1.00 0.00 C
ATOM 3887 H ILE A 415 17.401 73.491 -14.381 1.00 0.00 H
ATOM 3888 HA ILE A 415 15.291 71.644 -13.494 1.00 0.00 H
ATOM 3889 HB ILE A 415 15.894 74.311 -12.103 1.00 0.00 H
ATOM 3890 1HG1 ILE A 415 16.306 71.457 -11.070 1.00 0.00 H
ATOM 3891 2HG1 ILE A 415 17.597 72.634 -11.409 1.00 0.00 H
ATOM 3892 1HG2 ILE A 415 14.165 73.636 -10.536 1.00 0.00 H
ATOM 3893 2HG2 ILE A 415 13.551 73.797 -12.198 1.00 0.00 H
ATOM 3894 3HG2 ILE A 415 13.847 72.182 -11.512 1.00 0.00 H
ATOM 3895 1HD1 ILE A 415 17.174 72.442 -9.021 1.00 0.00 H
ATOM 3896 2HD1 ILE A 415 16.761 74.071 -9.606 1.00 0.00 H
ATOM 3897 3HD1 ILE A 415 15.470 72.894 -9.267 1.00 0.00 H
ATOM 3898 N THR A 416 13.675 73.111 -14.833 1.00 0.00 N
ATOM 3899 CA THR A 416 12.721 73.901 -15.601 1.00 0.00 C
ATOM 3900 C THR A 416 11.307 73.477 -15.157 1.00 0.00 C
ATOM 3901 O THR A 416 11.022 72.281 -15.126 1.00 0.00 O
ATOM 3902 CB THR A 416 12.979 73.664 -17.098 1.00 0.00 C
ATOM 3903 CG2 THR A 416 12.220 74.674 -17.961 1.00 0.00 C
ATOM 3904 OG1 THR A 416 14.364 73.764 -17.385 1.00 0.00 O
ATOM 3905 H THR A 416 13.367 72.181 -14.588 1.00 0.00 H
ATOM 3906 HA THR A 416 12.912 74.962 -15.438 1.00 0.00 H
ATOM 3907 HB THR A 416 12.668 72.654 -17.365 1.00 0.00 H
ATOM 3908 1HG2 THR A 416 12.424 74.478 -19.014 1.00 0.00 H
ATOM 3909 2HG2 THR A 416 11.150 74.580 -17.776 1.00 0.00 H
ATOM 3910 3HG2 THR A 416 12.545 75.684 -17.710 1.00 0.00 H
ATOM 3911 HG1 THR A 416 14.509 73.614 -18.322 1.00 0.00 H
ATOM 3912 N GLN A 417 10.433 74.414 -14.777 1.00 0.00 N
ATOM 3913 CA GLN A 417 9.223 74.136 -14.004 1.00 0.00 C
ATOM 3914 C GLN A 417 7.995 74.820 -14.611 1.00 0.00 C
ATOM 3915 O GLN A 417 8.070 75.974 -15.025 1.00 0.00 O
ATOM 3916 CB GLN A 417 9.413 74.643 -12.566 1.00 0.00 C
ATOM 3917 CG GLN A 417 10.359 73.733 -11.778 1.00 0.00 C
ATOM 3918 CD GLN A 417 10.778 74.361 -10.455 1.00 0.00 C

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ATOM   3919  NE2 GLN A 417      9.935  74.312  -9.435  1.00  0.00           N
ATOM   3920  OE1 GLN A 417     11.872  74.897 -10.336  1.00  0.00           O
ATOM   3921  H   GLN A 417     10.589  75.380 -15.024  1.00  0.00           H
ATOM   3922  HA  GLN A 417      9.047  73.061 -13.977  1.00  0.00           H
ATOM   3923  1HB GLN A 417      9.836  75.647 -12.587  1.00  0.00           H
ATOM   3924  2HB GLN A 417      8.449  74.665 -12.058  1.00  0.00           H
ATOM   3925  1HG GLN A 417      9.860  72.787 -11.564  1.00  0.00           H
ATOM   3926  2HG GLN A 417     11.257  73.544 -12.366  1.00  0.00           H
ATOM   3927  1HE2 GLN A 417    10.191  74.722  -8.548  1.00  0.00           H
ATOM   3928  2HE2 GLN A 417     9.035  73.866  -9.543  1.00  0.00           H
ATOM   3929  N   LYS A 418      6.845  74.140 -14.602  1.00  0.00           N
ATOM   3930  CA  LYS A 418      5.549  74.715 -14.938  1.00  0.00           C
ATOM   3931  C   LYS A 418      4.470  74.063 -14.068  1.00  0.00           C
ATOM   3932  O   LYS A 418      4.578  72.883 -13.737  1.00  0.00           O
ATOM   3933  CB  LYS A 418      5.212  74.468 -16.414  1.00  0.00           C
ATOM   3934  CG  LYS A 418      6.108  75.244 -17.387  1.00  0.00           C
ATOM   3935  CD  LYS A 418      5.523  75.122 -18.805  1.00  0.00           C
ATOM   3936  CE  LYS A 418      6.241  76.046 -19.797  1.00  0.00           C
ATOM   3937  NZ  LYS A 418      7.656  75.685 -19.975  1.00  0.00           N1+
ATOM   3938  H   LYS A 418      6.839  73.161 -14.353  1.00  0.00           H
ATOM   3939  HA  LYS A 418      5.567  75.788 -14.748  1.00  0.00           H
ATOM   3940  1HB LYS A 418      5.326  73.408 -16.642  1.00  0.00           H
ATOM   3941  2HB LYS A 418      4.183  74.772 -16.608  1.00  0.00           H
ATOM   3942  1HG LYS A 418      6.144  76.293 -17.092  1.00  0.00           H
ATOM   3943  2HG LYS A 418      7.115  74.826 -17.366  1.00  0.00           H
ATOM   3944  1HD LYS A 418      5.629  74.096 -19.156  1.00  0.00           H
ATOM   3945  2HD LYS A 418      4.468  75.393 -18.788  1.00  0.00           H
ATOM   3946  1HE LYS A 418      5.754  75.984 -20.770  1.00  0.00           H
ATOM   3947  2HE LYS A 418      6.199  77.073 -19.434  1.00  0.00           H
ATOM   3948  1HZ LYS A 418      8.086  76.318 -20.634  1.00  0.00           H
ATOM   3949  2HZ LYS A 418      8.135  75.748 -19.087  1.00  0.00           H
ATOM   3950  3HZ LYS A 418      7.722  74.740 -20.325  1.00  0.00           H
ATOM   3951  N   VAL A 419      3.415  74.809 -13.731  1.00  0.00           N
ATOM   3952  CA  VAL A 419      2.330  74.351 -12.874  1.00  0.00           C
ATOM   3953  C   VAL A 419      1.025  74.941 -13.425  1.00  0.00           C
ATOM   3954  O   VAL A 419      0.990  76.125 -13.764  1.00  0.00           O
ATOM   3955  CB  VAL A 419      2.571  74.803 -11.418  1.00  0.00           C
ATOM   3956  CGI VAL A 419      1.585  74.124 -10.460  1.00  0.00           C
ATOM   3957  CG2 VAL A 419      3.993  74.506 -10.915  1.00  0.00           C
ATOM   3958  H   VAL A 419      3.335  75.755 -14.074  1.00  0.00           H
ATOM   3959  HA  VAL A 419      2.304  73.261 -12.871  1.00  0.00           H
ATOM   3960  HB  VAL A 419      2.466  75.886 -11.350  1.00  0.00           H
ATOM   3961  1HG1 VAL A 419     1.777  74.459  -9.441  1.00  0.00           H
ATOM   3962  2HG1 VAL A 419     0.565  74.385 -10.742  1.00  0.00           H
ATOM   3963  3HG1 VAL A 419     1.711  73.042 -10.516  1.00  0.00           H
ATOM   3964  1HG2 VAL A 419     4.094  74.849  -9.886  1.00  0.00           H
ATOM   3965  2HG2 VAL A 419     4.178  73.432 -10.960  1.00  0.00           H
ATOM   3966  3HG2 VAL A 419     4.717  75.025 -11.543  1.00  0.00           H
ATOM   3967  N   VAL A 420     -0.036  74.140 -13.519  1.00  0.00           N
ATOM   3968  CA  VAL A 420     -1.347  74.545 -14.013  1.00  0.00           C
ATOM   3969  C   VAL A 420     -2.414  73.741 -13.265  1.00  0.00           C
ATOM   3970  O   VAL A 420     -2.167  72.596 -12.896  1.00  0.00           O
ATOM   3971  CB  VAL A 420     -1.454  74.318 -15.536  1.00  0.00           C
ATOM   3972  CGI VAL A 420     -0.665  75.370 -16.326  1.00  0.00           C
ATOM   3973  CG2 VAL A 420     -0.990  72.920 -15.970  1.00  0.00           C
ATOM   3974  H   VAL A 420      0.035  73.172 -13.237  1.00  0.00           H
ATOM   3975  HA  VAL A 420     -1.476  75.617 -13.866  1.00  0.00           H
ATOM   3976  HB  VAL A 420     -2.503  74.317 -15.831  1.00  0.00           H
ATOM   3977  1HG1 VAL A 420    -0.766  75.174 -17.394  1.00  0.00           H
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ATOM   3978 2HG1 VAL A 420     -1.055  76.362 -16.100  1.00  0.00        H
ATOM   3979 3HG1 VAL A 420      0.387  75.321 -16.046  1.00  0.00        H
ATOM   3980 1HG2 VAL A 420     -1.090  72.823 -17.051  1.00  0.00        H
ATOM   3981 2HG2 VAL A 420      0.053  72.778 -15.688  1.00  0.00        H
ATOM   3982 3HG2 VAL A 420     -1.604  72.164 -15.480  1.00  0.00        H
ATOM   3983  N   TRP A 421    -3.594  74.320 -13.036  1.00  0.00        N
ATOM   3984  CA  TRP A 421    -4.707  73.587 -12.446  1.00  0.00        C
ATOM   3985  C   TRP A 421    -5.363  72.772 -13.560  1.00  0.00        C
ATOM   3986  O   TRP A 421    -5.759  73.346 -14.573  1.00  0.00        O
ATOM   3987  CB  TRP A 421    -5.701  74.560 -11.796  1.00  0.00        C
ATOM   3988  CG  TRP A 421    -6.680  73.970 -10.819  1.00  0.00        C
ATOM   3989  CD1 TRP A 421    -7.447  72.870 -11.010  1.00  0.00        C
ATOM   3990  CD2 TRP A 421    -7.021  74.451 -9.482  1.00  0.00        C
ATOM   3991  CE2 TRP A 421    -7.995  73.572  -8.919  1.00  0.00        C
ATOM   3992  CE3 TRP A 421    -6.623  75.544  -8.679  1.00  0.00        C
ATOM   3993  NE1 TRP A 421    -8.207  72.619  -9.889  1.00  0.00        N
ATOM   3994  CZ2 TRP A 421    -8.530  73.765  -7.636  1.00  0.00        C
ATOM   3995  CZ3 TRP A 421    -7.159  75.751 -7.395  1.00  0.00        C
ATOM   3996  CH2 TRP A 421    -8.114  74.864  -6.872  1.00  0.00        C
ATOM   3997  H   TRP A 421    -3.735  75.291 -13.274  1.00  0.00        H
ATOM   3998  HA  TRP A 421    -4.338  72.954 -11.639  1.00  0.00        H
ATOM   3999 1HB  TRP A 421    -5.153  75.324 -11.243  1.00  0.00        H
ATOM   4000 2HB  TRP A 421    -6.303  75.036 -12.570  1.00  0.00        H
ATOM   4001  HD1 TRP A 421    -7.397  72.333 -11.945  1.00  0.00        H
ATOM   4002  HE3 TRP A 421    -5.890  76.246  -9.048  1.00  0.00        H
ATOM   4003  HE1 TRP A 421    -8.819  71.816  -9.863  1.00  0.00        H
ATOM   4004  HZ2 TRP A 421    -9.257  73.070  -7.244  1.00  0.00        H
ATOM   4005  HZ3 TRP A 421    -6.837  76.596  -6.805  1.00  0.00        H
ATOM   4006  HH2 TRP A 421    -8.527  75.024  -5.887  1.00  0.00        H
ATOM   4007  N   VAL A 422    -5.481  71.456 -13.386  1.00  0.00        N
ATOM   4008  CA  VAL A 422    -6.138  70.560 -14.328  1.00  0.00        C
ATOM   4009  C   VAL A 422    -6.677  69.397 -13.496  1.00  0.00        C
ATOM   4010  O   VAL A 422    -5.898  68.751 -12.796  1.00  0.00        O
ATOM   4011  CB  VAL A 422    -5.141  70.046 -15.390  1.00  0.00        C
ATOM   4012  CGI VAL A 422    -5.822  69.063 -16.351  1.00  0.00        C
ATOM   4013  CG2 VAL A 422    -4.514  71.165 -16.233  1.00  0.00        C
ATOM   4014  H   VAL A 422    -5.101  71.020 -12.558  1.00  0.00        H
ATOM   4015  HA  VAL A 422    -6.947  71.091 -14.831  1.00  0.00        H
ATOM   4016  HB  VAL A 422    -4.301  69.559 -14.895  1.00  0.00        H
ATOM   4017 1HG1 VAL A 422    -5.099  68.715 -17.089  1.00  0.00        H
ATOM   4018 2HG1 VAL A 422    -6.205  68.211 -15.789  1.00  0.00        H
ATOM   4019 3HG1 VAL A 422    -6.647  69.563 -16.858  1.00  0.00        H
ATOM   4020 1HG2 VAL A 422    -3.825  70.733 -16.958  1.00  0.00        H
ATOM   4021 2HG2 VAL A 422    -5.299  71.709 -16.758  1.00  0.00        H
ATOM   4022 3HG2 VAL A 422    -3.972  71.851 -15.581  1.00  0.00        H
ATOM   4023  N   GLU A 423    -7.981  69.130 -13.572  1.00  0.00        N
ATOM   4024  CA  GLU A 423    -8.638  68.137 -12.736  1.00  0.00        C
ATOM   4025  C   GLU A 423    -8.498  66.732 -13.317  1.00  0.00        C
ATOM   4026  O   GLU A 423    -8.254  66.566 -14.510  1.00  0.00        O
ATOM   4027  CB  GLU A 423   -10.124  68.487 -12.583  1.00  0.00        C
ATOM   4028  CG  GLU A 423   -10.326  69.693 -11.658  1.00  0.00        C
ATOM   4029  CD  GLU A 423    -9.865  69.403 -10.238  1.00  0.00        C
ATOM   4030  OE1 GLU A 423    -9.641  68.212  -9.923  1.00  0.00        O
ATOM   4031  OE2 GLU A 423    -9.687  70.391  -9.499  1.00  0.00        Ol-
ATOM   4032  H   GLU A 423    -8.561  69.627 -14.234  1.00  0.00        H
ATOM   4033  HA  GLU A 423    -8.212  68.167 -11.733  1.00  0.00        H
ATOM   4034 1HB  GLU A 423   -10.544  68.727 -13.559  1.00  0.00        H
ATOM   4035 2HB  GLU A 423   -10.656  67.635 -12.159  1.00  0.00        H
ATOM   4036 1HG  GLU A 423    -9.754  70.541 -12.036  1.00  0.00        H
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ATOM 4037 2HG GLU A 423 -11.384 69.954 -11.626 1.00 0.00 H
ATOM 4038 N GLU A 424 -8.654 65.731 -12.447 1.00 0.00 N
ATOM 4039 CA GLU A 424 -8.469 64.305 -12.682 1.00 0.00 C
ATOM 4040 C GLU A 424 -8.888 63.825 -14.079 1.00 0.00 C
ATOM 4041 O GLU A 424 -8.233 62.953 -14.649 1.00 0.00 O
ATOM 4042 CB GLU A 424 -9.251 63.507 -11.629 1.00 0.00 C
ATOM 4043 CG GLU A 424 -8.908 63.856 -10.175 1.00 0.00 C
ATOM 4044 CD GLU A 424 -7.475 63.517 -9.831 1.00 0.00 C
ATOM 4045 OE1 GLU A 424 -7.230 62.366 -9.421 1.00 0.00 O
ATOM 4046 OE2 GLU A 424 -6.620 64.423 -9.823 1.00 0.00 Ol-
ATOM 4047 H GLU A 424 -8.934 65.927 -11.497 1.00 0.00 H
ATOM 4048 HA GLU A 424 -7.423 64.042 -12.520 1.00 0.00 H
ATOM 4049 1HB GLU A 424 -10.319 63.689 -11.754 1.00 0.00 H
ATOM 4050 2HB GLU A 424 -9.048 62.443 -11.754 1.00 0.00 H
ATOM 4051 IHG GLU A 424 -9.051 64.925 -10.014 1.00 0.00 H
ATOM 4052 2HG GLU A 424 -9.559 63.298 -9.503 1.00 0.00 H
ATOM 4053 N SER A 425 -10.017 64.315 -14.591 1.00 0.00 N
ATOM 4054 CA SER A 425 -10.503 63.979 -15.914 1.00 0.00 C
ATOM 4055 C SER A 425 -9.444 64.333 -16.955 1.00 0.00 C
ATOM 4056 O SER A 425 -9.004 63.502 -17.751 1.00 0.00 O
ATOM 4057 CB SER A 425 -11.790 64.777 -16.168 1.00 0.00 C
ATOM 4058 OG SER A 425 -11.685 66.090 -15.636 1.00 0.00 O
ATOM 4059 H SER A 425 -10.581 64.955 -14.049 1.00 0.00 H
ATOM 4060 HA SER A 425 -10.722 62.912 -15.961 1.00 0.00 H
ATOM 4061 1HB SER A 425 -11.969 64.848 -17.241 1.00 0.00 H
ATOM 4062 2HB SER A 425 -12.631 64.273 -15.692 1.00 0.00 H
ATOM 4063 HG SER A 425 -12.499 66.570 -15.805 1.00 0.00 H
ATOM 4064 N ASP A 426 -9.071 65.603 -16.951 1.00 0.00 N
ATOM 4065 CA ASP A 426 -8.343 66.239 -18.024 1.00 0.00 C
ATOM 4066 C ASP A 426 -6.851 66.160 -17.747 1.00 0.00 C
ATOM 4067 O ASP A 426 -6.035 66.545 -18.583 1.00 0.00 O
ATOM 4068 CB ASP A 426 -8.869 67.655 -18.235 1.00 0.00 C
ATOM 4069 CG ASP A 426 -10.282 67.553 -18.775 1.00 0.00 C
ATOM 4070 OD1 ASP A 426 -10.398 67.429 -20.014 1.00 0.00 O
ATOM 4071 OD2 ASP A 426 -11.209 67.502 -17.938 1.00 0.00 Ol-
ATOM 4072 H ASP A 426 -9.293 66.193 -16.162 1.00 0.00 H
ATOM 4073 HA ASP A 426 -8.648 65.806 -18.977 1.00 0.00 H
ATOM 4074 1HB ASP A 426 -8.866 68.189 -17.285 1.00 0.00 H
ATOM 4075 2HB ASP A 426 -8.230 68.178 -18.947 1.00 0.00 H
ATOM 4076 N LYS A 427 -6.485 65.551 -16.618 1.00 0.00 N
ATOM 4077 CA LYS A 427 -5.171 64.966 -16.454 1.00 0.00 C
ATOM 4078 C LYS A 427 -5.010 63.752 -17.389 1.00 0.00 C
ATOM 4079 O LYS A 427 -3.941 63.147 -17.413 1.00 0.00 O
ATOM 4080 CB LYS A 427 -4.909 64.577 -14.991 1.00 0.00 C
ATOM 4081 CG LYS A 427 -4.964 65.747 -13.995 1.00 0.00 C
ATOM 4082 CD LYS A 427 -4.552 65.272 -12.591 1.00 0.00 C
ATOM 4083 CE LYS A 427 -4.792 66.348 -11.521 1.00 0.00 C
ATOM 4084 NZ LYS A 427 -4.477 65.863 -10.168 1.00 0.00 N1+
ATOM 4085 H LYS A 427 -7.133 65.488 -15.846 1.00 0.00 H
ATOM 4086 HA LYS A 427 -4.410 65.726 -16.632 1.00 0.00 H
ATOM 4087 1HB LYS A 427 -5.657 63.854 -14.668 1.00 0.00 H
ATOM 4088 2HB LYS A 427 -3.916 64.136 -14.904 1.00 0.00 H
ATOM 4089 IHG LYS A 427 -4.282 66.533 -14.320 1.00 0.00 H
ATOM 4090 2HG LYS A 427 -5.979 66.142 -13.954 1.00 0.00 H
ATOM 4091 1HD LYS A 427 -5.132 64.390 -12.320 1.00 0.00 H
ATOM 4092 2HD LYS A 427 -3.491 65.023 -12.588 1.00 0.00 H
ATOM 4093 1HE LYS A 427 -4.161 67.213 -11.727 1.00 0.00 H
ATOM 4094 2HE LYS A 427 -5.839 66.651 -11.538 1.00 0.00 H
ATOM 4095 1HZ LYS A 427 -4.648 66.599 -9.497 1.00 0.00 H

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ATOM   4096 2HZ  LYS A 427      -5.061   65.068  -9.951   1.00  0.00           H
ATOM   4097 3HZ  LYS A 427      -3.506   65.589 -10.126   1.00  0.00           H
ATOM   4098  N   ARG A 428      -6.045   63.378 -18.156   1.00  0.00           N
ATOM   4099  CA  ARG A 428      -5.901   62.563 -19.353   1.00  0.00           C
ATOM   4100  C   ARG A 428      -5.848   63.480 -20.580   1.00  0.00           C
ATOM   4101  O   ARG A 428      -4.893   63.427 -21.349   1.00  0.00           O
ATOM   4102  CB  ARG A 428      -7.035   61.537 -19.494   1.00  0.00           C
ATOM   4103  CG  ARG A 428      -7.023   60.491 -18.371   1.00  0.00           C
ATOM   4104  CD  ARG A 428      -7.880   59.279 -18.768   1.00  0.00           C
ATOM   4105  NE  ARG A 428      -7.865   58.239 -17.723   1.00  0.00           N
ATOM   4106  CZ  ARG A 428      -8.117   56.932 -17.904   1.00  0.00           C
ATOM   4107  NH1 ARG A 428      -8.430   56.443 -19.103   1.00  0.00           N1+
ATOM   4108  NH2 ARG A 428      -8.033   56.092 -16.883   1.00  0.00           N
ATOM   4109  H   ARG A 428      -6.983   63.663 -17.913   1.00  0.00           H
ATOM   4110  HA  ARG A 428      -5.008   61.944 -19.267   1.00  0.00           H
ATOM   4111 1HB  ARG A 428      -7.996   62.050 -19.464   1.00  0.00           H
ATOM   4112 2HB  ARG A 428      -6.934   61.011 -20.443   1.00  0.00           H
ATOM   4113 1HG  ARG A 428      -5.999   60.162 -18.191   1.00  0.00           H
ATOM   4114 2HG  ARG A 428      -7.427   60.932 -17.459   1.00  0.00           H
ATOM   4115 1HD  ARG A 428      -8.911   59.597 -18.923   1.00  0.00           H
ATOM   4116 2HD  ARG A 428      -7.492   58.845 -19.690   1.00  0.00           H
ATOM   4117  HE  ARG A 428      -7.641   58.587 -16.802   1.00  0.00           H
ATOM   4118 1HH1 ARG A 428      -8.615   55.456 -19.213   1.00  0.00           H
ATOM   4119 2HH1 ARG A 428      -8.484   57.058 -19.902   1.00  0.00           H
ATOM   4120 1HH2 ARG A 428      -8.222   55.109 -17.021   1.00  0.00           H
ATOM   4121 2HH2 ARG A 428      -7.780   56.434 -15.967   1.00  0.00           H
ATOM   4122  N   SER A 429      -6.879   64.297 -20.794   1.00  0.00           N
ATOM   4123  CA  SER A 429      -7.008   65.135 -21.976   1.00  0.00           C
ATOM   4124  C   SER A 429      -5.747   65.967 -22.254   1.00  0.00           C
ATOM   4125  O   SER A 429      -5.261   66.020 -23.382   1.00  0.00           O
ATOM   4126  CB  SER A 429      -8.229   66.041 -21.799   1.00  0.00           C
ATOM   4127  OG  SER A 429      -9.324   65.301 -21.285   1.00  0.00           O
ATOM   4128  H   SER A 429      -7.625   64.357 -20.116   1.00  0.00           H
ATOM   4129  HA  SER A 429      -7.247   64.514 -22.839   1.00  0.00           H
ATOM   4130 1HB  SER A 429      -7.988   66.846 -21.104   1.00  0.00           H
ATOM   4131 2HB  SER A 429      -8.510   66.467 -22.762   1.00  0.00           H
ATOM   4132  HG  SER A 429     -10.081   65.882 -21.180   1.00  0.00           H
ATOM   4133  N   PHE A 430      -5.236   66.650 -21.230   1.00  0.00           N
ATOM   4134  CA  PHE A 430      -4.116   67.571 -21.357   1.00  0.00           C
ATOM   4135  C   PHE A 430      -2.817   66.766 -21.492   1.00  0.00           C
ATOM   4136  O   PHE A 430      -1.821   67.237 -22.034   1.00  0.00           O
ATOM   4137  CB  PHE A 430      -4.095   68.475 -20.111   1.00  0.00           C
ATOM   4138  CG  PHE A 430      -3.428   69.834 -20.252   1.00  0.00           C
ATOM   4139  CD1 PHE A 430      -4.198   71.010 -20.143   1.00  0.00           C
ATOM   4140  CD2 PHE A 430      -2.040   69.957 -20.466   1.00  0.00           C
ATOM   4141  CE1 PHE A 430      -3.597   72.277 -20.240   1.00  0.00           C
ATOM   4142  CE2 PHE A 430      -1.437   71.222 -20.573   1.00  0.00           C
ATOM   4143  CZ  PHE A 430      -2.215   72.385 -20.458   1.00  0.00           C
ATOM   4144  H   PHE A 430      -5.627   66.541 -20.305   1.00  0.00           H
ATOM   4145  HA  PHE A 430      -4.269   68.212 -22.225   1.00  0.00           H
ATOM   4146 1HB  PHE A 430      -5.118   68.684 -19.796   1.00  0.00           H
ATOM   4147 2HB  PHE A 430      -3.562   67.972 -19.305   1.00  0.00           H
ATOM   4148  HD1 PHE A 430      -5.264   70.945 -19.982   1.00  0.00           H
ATOM   4149  HD2 PHE A 430      -1.426   69.073 -20.550   1.00  0.00           H
ATOM   4150  HE1 PHE A 430      -4.200   73.169 -20.148   1.00  0.00           H
ATOM   4151  HE2 PHE A 430      -0.373   71.300 -20.744   1.00  0.00           H
ATOM   4152  HZ  PHE A 430      -1.754   73.359 -20.536   1.00  0.00           H
ATOM   4153  N   LEU A 431      -2.812   65.547 -20.954   1.00  0.00           N
ATOM   4154  CA  LEU A 431      -1.630   64.705 -20.869   1.00  0.00           C
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ATOM 4155 C LEU A 431 -1.194 64.244 -22.265 1.00 0.00 C
ATOM 4156 O LEU A 431 -0.060 63.801 -22.444 1.00 0.00 O
ATOM 4157 CB LEU A 431 -1.951 63.546 -19.909 1.00 0.00 C
ATOM 4158 CG LEU A 431 -0.852 62.510 -19.653 1.00 0.00 C
ATOM 4159 CD1 LEU A 431 0.341 63.123 -18.923 1.00 0.00 C
ATOM 4160 CD2 LEU A 431 -1.409 61.370 -18.792 1.00 0.00 C
ATOM 4161 H LEU A 431 -3.664 65.159 -20.576 1.00 0.00 H
ATOM 4162 HA LEU A 431 -0.842 65.238 -20.338 1.00 0.00 H
ATOM 4163 1HB LEU A 431 -2.201 63.947 -18.927 1.00 0.00 H
ATOM 4164 2HB LEU A 431 -2.797 62.977 -20.295 1.00 0.00 H
ATOM 4165 HG LEU A 431 -0.502 62.107 -20.604 1.00 0.00 H
ATOM 4166 1HD1 LEU A 431 1.100 62.358 -18.759 1.00 0.00 H
ATOM 4167 2HD1 LEU A 431 0.762 63.928 -19.526 1.00 0.00 H
ATOM 4168 3HD1 LEU A 431 0.014 63.522 -17.963 1.00 0.00 H
ATOM 4169 1HD2 LEU A 431 -0.626 60.634 -18.611 1.00 0.00 H
ATOM 4170 2HD2 LEU A 431 -1.757 61.771 -17.840 1.00 0.00 H
ATOM 4171 3HD2 LEU A 431 -2.241 60.895 -19.311 1.00 0.00 H
ATOM 4172 N LEU A 432 -2.092 64.336 -23.248 1.00 0.00 N
ATOM 4173 CA LEU A 432 -1.822 63.954 -24.622 1.00 0.00 C
ATOM 4174 C LEU A 432 -0.555 64.632 -25.149 1.00 0.00 C
ATOM 4175 O LEU A 432 0.349 63.940 -25.620 1.00 0.00 O
ATOM 4176 CB LEU A 432 -3.027 64.266 -25.521 1.00 0.00 C
ATOM 4177 CG LEU A 432 -4.257 63.385 -25.238 1.00 0.00 C
ATOM 4178 CD1 LEU A 432 -5.444 63.902 -26.060 1.00 0.00 C
ATOM 4179 CD2 LEU A 432 -4.009 61.916 -25.610 1.00 0.00 C
ATOM 4180 H LEU A 432 -3.018 64.689 -23.054 1.00 0.00 H
ATOM 4181 HA LEU A 432 -1.757 62.868 -24.691 1.00 0.00 H
ATOM 4182 1HB LEU A 432 -3.331 65.302 -25.374 1.00 0.00 H
ATOM 4183 2HB LEU A 432 -2.753 64.113 -26.565 1.00 0.00 H
ATOM 4184 HG LEU A 432 -4.499 63.427 -24.176 1.00 0.00 H
ATOM 4185 1HD1 LEU A 432 -6.319 63.283 -25.865 1.00 0.00 H
ATOM 4186 2HD1 LEU A 432 -5.659 64.933 -25.780 1.00 0.00 H
ATOM 4187 3HD1 LEU A 432 -5.198 63.859 -27.121 1.00 0.00 H
ATOM 4188 1HD2 LEU A 432 -4.902 61.330 -25.395 1.00 0.00 H
ATOM 4189 2HD2 LEU A 432 -3.776 61.844 -26.672 1.00 0.00 H
ATOM 4190 3HD2 LEU A 432 -3.172 61.530 -25.028 1.00 0.00 H
ATOM 4191 N ASP A 433 -0.487 65.966 -25.115 1.00 0.00 N
ATOM 4192 CA ASP A 433 0.691 66.680 -25.604 1.00 0.00 C
ATOM 4193 C ASP A 433 1.906 66.236 -24.800 1.00 0.00 C
ATOM 4194 O ASP A 433 2.933 65.840 -25.350 1.00 0.00 O
ATOM 4195 CB ASP A 433 0.541 68.198 -25.482 1.00 0.00 C
ATOM 4196 CG ASP A 433 1.872 68.860 -25.824 1.00 0.00 C
ATOM 4197 OD1 ASP A 433 2.156 68.973 -27.035 1.00 0.00 O
ATOM 4198 OD2 ASP A 433 2.604 69.205 -24.872 1.00 0.00 Ol-
ATOM 4199 H ASP A 433 -1.259 66.502 -24.746 1.00 0.00 H
ATOM 4200 HA ASP A 433 0.836 66.462 -26.662 1.00 0.00 H
ATOM 4201 1HB ASP A 433 -0.228 68.544 -26.172 1.00 0.00 H
ATOM 4202 2HB ASP A 433 0.255 68.454 -24.462 1.00 0.00 H
ATOM 4203 N LEU A 434 1.760 66.290 -23.479 1.00 0.00 N
ATOM 4204 CA LEU A 434 2.867 66.138 -22.559 1.00 0.00 C
ATOM 4205 C LEU A 434 3.579 64.794 -22.760 1.00 0.00 C
ATOM 4206 O LEU A 434 4.769 64.672 -22.452 1.00 0.00 O
ATOM 4207 CB LEU A 434 2.371 66.285 -21.113 1.00 0.00 C
ATOM 4208 CG LEU A 434 1.598 67.580 -20.802 1.00 0.00 C
ATOM 4209 CD1 LEU A 434 1.275 67.611 -19.305 1.00 0.00 C
ATOM 4210 CD2 LEU A 434 2.358 68.863 -21.159 1.00 0.00 C
ATOM 4211 H LEU A 434 0.845 66.442 -23.078 1.00 0.00 H
ATOM 4212 HA LEU A 434 3.558 66.972 -22.680 1.00 0.00 H
ATOM 4213 1HB LEU A 434 1.698 65.462 -20.874 1.00 0.00 H

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ATOM   4214 2HB  LEU A 434      3.223  66.266 -20.433  1.00  0.00           H
ATOM   4215  HG  LEU A 434      0.683  67.609 -21.394  1.00  0.00           H
ATOM   4216 1HD1 LEU A 434      0.728  68.524 -19.069  1.00  0.00           H
ATOM   4217 2HD1 LEU A 434      0.666  66.745 -19.046  1.00  0.00           H
ATOM   4218 3HD1 LEU A 434      2.203  67.587 -18.732  1.00  0.00           H
ATOM   4219 1HD2 LEU A 434      1.746  69.729 -20.909  1.00  0.00           H
ATOM   4220 2HD2 LEU A 434      3.290  68.902 -20.596  1.00  0.00           H
ATOM   4221 3HD2 LEU A 434      2.579  68.869 -22.226  1.00  0.00           H
ATOM   4222  N   LEU A 435      2.849  63.788 -23.254  1.00  0.00           N
ATOM   4223  CA  LEU A 435      3.371  62.470 -23.567  1.00  0.00           C
ATOM   4224  C   LEU A 435      3.720  62.343 -25.047  1.00  0.00           C
ATOM   4225  O   LEU A 435      4.697  61.673 -25.378  1.00  0.00           O
ATOM   4226  CB  LEU A 435      2.366  61.384 -23.187  1.00  0.00           C
ATOM   4227  CG  LEU A 435      2.093  61.305 -21.681  1.00  0.00           C
ATOM   4228  CD1 LEU A 435      1.127  60.148 -21.450  1.00  0.00           C
ATOM   4229  CD2 LEU A 435      3.354  61.070 -20.848  1.00  0.00           C
ATOM   4230  H   LEU A 435      1.864  63.919 -23.433  1.00  0.00           H
ATOM   4231  HA  LEU A 435      4.252  62.273 -22.956  1.00  0.00           H
ATOM   4232 1HB  LEU A 435      1.415  61.581 -23.682  1.00  0.00           H
ATOM   4233 2HB  LEU A 435      2.745  60.412 -23.502  1.00  0.00           H
ATOM   4234  HG  LEU A 435      1.656  62.245 -21.340  1.00  0.00           H
ATOM   4235 1HD1 LEU A 435      0.909  60.062 -20.386  1.00  0.00           H
ATOM   4236 2HD1 LEU A 435      0.201  60.331 -21.996  1.00  0.00           H
ATOM   4237 3HD1 LEU A 435      1.579  59.221 -21.804  1.00  0.00           H
ATOM   4238 1HD2 LEU A 435      3.090  61.025 -19.791  1.00  0.00           H
ATOM   4239 2HD2 LEU A 435      3.818  60.130 -21.147  1.00  0.00           H
ATOM   4240 3HD2 LEU A 435      4.056  61.889 -21.011  1.00  0.00           H
ATOM   4241  N   ASN A 436      2.972  62.970 -25.954  1.00  0.00           N
ATOM   4242  CA  ASN A 436      3.369  63.012 -27.362  1.00  0.00           C
ATOM   4243  C   ASN A 436      4.712  63.733 -27.484  1.00  0.00           C
ATOM   4244  O   ASN A 436      5.469  63.523 -28.430  1.00  0.00           O
ATOM   4245  CB  ASN A 436      2.304  63.684 -28.236  1.00  0.00           C
ATOM   4246  CG  ASN A 436      1.272  62.670 -28.711  1.00  0.00           C
ATOM   4247 ND2 ASN A 436      0.194  62.488 -27.962  1.00  0.00           N
ATOM   4248 OD1 ASN A 436      1.464  62.018 -29.732  1.00  0.00           O
ATOM   4249  H   ASN A 436      2.116  63.426 -25.674  1.00  0.00           H
ATOM   4250  HA  ASN A 436      3.409  61.998 -27.759  1.00  0.00           H
ATOM   4251 1HB  ASN A 436      1.796  64.457 -27.660  1.00  0.00           H
ATOM   4252 2HB  ASN A 436      2.780  64.134 -29.107  1.00  0.00           H
ATOM   4253 1HD2 ASN A 436     -0.512  61.823 -28.246  1.00  0.00           H
ATOM   4254 2HD2 ASN A 436      0.078  63.012 -27.107  1.00  0.00           H
ATOM   4255  N   ALA A 437      5.038  64.556 -26.491  1.00  0.00           N
ATOM   4256  CA  ALA A 437      6.305  65.234 -26.371  1.00  0.00           C
ATOM   4257  C   ALA A 437      7.431  64.266 -25.982  1.00  0.00           C
ATOM   4258  O   ALA A 437      8.570  64.712 -25.811  1.00  0.00           O
ATOM   4259  CB  ALA A 437      6.175  66.378 -25.360  1.00  0.00           C
ATOM   4260  H   ALA A 437      4.375  64.743 -25.751  1.00  0.00           H
ATOM   4261  HA  ALA A 437      6.531  65.751 -27.303  1.00  0.00           H
ATOM   4262 1HB  ALA A 437      7.131  66.892 -25.267  1.00  0.00           H
ATOM   4263 2HB  ALA A 437      5.416  67.082 -25.703  1.00  0.00           H
ATOM   4264 3HB  ALA A 437      5.884  65.975 -24.390  1.00  0.00           H
ATOM   4265  N   THR A 438      7.162  62.963 -25.855  1.00  0.00           N
ATOM   4266  CA  THR A 438      8.188  61.939 -25.727  1.00  0.00           C
ATOM   4267  C   THR A 438      8.827  61.725 -27.105  1.00  0.00           C
ATOM   4268  O   THR A 438      8.636  60.713 -27.774  1.00  0.00           O
ATOM   4269  CB  THR A 438      7.588  60.659 -25.124  1.00  0.00           C
ATOM   4270 CG2 THR A 438      8.672  59.665 -24.706  1.00  0.00           C
ATOM   4271 OG1 THR A 438      6.847  60.991 -23.966  1.00  0.00           O
ATOM   4272  H   THR A 438      6.204  62.644 -25.844  1.00  0.00           H
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ATOM   4273  HA  THR A 438      8.898  62.230 -24.952  1.00  0.00           H
ATOM   4274  HB  THR A 438      6.964  60.164 -25.868  1.00  0.00           H
ATOM   4275 1HG2 THR A 438      8.207  58.774 -24.285  1.00  0.00           H
ATOM   4276 2HG2 THR A 438      9.266  59.387 -25.576  1.00  0.00           H
ATOM   4277 3HG2 THR A 438      9.318  60.125 -23.958  1.00  0.00           H
ATOM   4278  HG1 THR A 438      6.471  60.194 -23.586  1.00  0.00           H
ATOM   4279  N   GLY A 439      9.619  62.710 -27.509  1.00  0.00           N
ATOM   4280  CA  GLY A 439     10.309  62.808 -28.776  1.00  0.00           C
ATOM   4281  C   GLY A 439     11.101  64.111 -28.688  1.00  0.00           C
ATOM   4282  O   GLY A 439     11.209  64.674 -27.600  1.00  0.00           O
ATOM   4283  H   GLY A 439      9.791  63.500 -26.904  1.00  0.00           H
ATOM   4284 1HA  GLY A 439     10.963  61.946 -28.901  1.00  0.00           H
ATOM   4285 2HA  GLY A 439      9.581  62.832 -29.586  1.00  0.00           H
ATOM   4286  N   LYS A 440     11.635  64.635 -29.791  1.00  0.00           N
ATOM   4287  CA  LYS A 440     12.697  65.636 -29.725  1.00  0.00           C
ATOM   4288  C   LYS A 440     13.908  64.908 -29.120  1.00  0.00           C
ATOM   4289  O   LYS A 440     14.251  63.834 -29.606  1.00  0.00           O
ATOM   4290  CB  LYS A 440     12.272  66.917 -28.958  1.00  0.00           C
ATOM   4291  CG  LYS A 440     10.885  67.469 -29.342  1.00  0.00           C
ATOM   4292  CD  LYS A 440     10.365  68.490 -28.308  1.00  0.00           C
ATOM   4293  CE  LYS A 440      9.430  67.879 -27.244  1.00  0.00           C
ATOM   4294  NZ  LYS A 440     10.053  66.802 -26.445  1.00  0.00           N1+
ATOM   4295  H   LYS A 440     11.307  64.340 -30.700  1.00  0.00           H
ATOM   4296  HA  LYS A 440     12.847  66.073 -30.712  1.00  0.00           H
ATOM   4297 1HB  LYS A 440     12.241  66.707 -27.889  1.00  0.00           H
ATOM   4298 2HB  LYS A 440     12.991  67.712 -29.151  1.00  0.00           H
ATOM   4299 1HG  LYS A 440     10.947  67.966 -30.310  1.00  0.00           H
ATOM   4300 2HG  LYS A 440     10.170  66.648 -29.400  1.00  0.00           H
ATOM   4301 1HD  LYS A 440     11.208  68.935 -27.779  1.00  0.00           H
ATOM   4302 2HD  LYS A 440      9.804  69.272 -28.819  1.00  0.00           H
ATOM   4303 1HE  LYS A 440      9.115  68.655 -26.547  1.00  0.00           H
ATOM   4304 2HE  LYS A 440      8.554  67.451 -27.732  1.00  0.00           H
ATOM   4305 1HZ  LYS A 440      9.386  66.452 -25.773  1.00  0.00           H
ATOM   4306 2HZ  LYS A 440     10.340  66.052 -27.057  1.00  0.00           H
ATOM   4307 3HZ  LYS A 440     10.860  67.167 -25.959  1.00  0.00           H
ATOM   4308  N   ASP A 441     14.483  65.421 -28.031  1.00  0.00           N
ATOM   4309  CA  ASP A 441     15.262  64.628 -27.093  1.00  0.00           C
ATOM   4310  C   ASP A 441     14.521  64.753 -25.762  1.00  0.00           C
ATOM   4311  O   ASP A 441     14.618  65.778 -25.087  1.00  0.00           O
ATOM   4312  CB  ASP A 441     16.688  65.179 -26.974  1.00  0.00           C
ATOM   4313  CG  ASP A 441     17.401  64.563 -25.784  1.00  0.00           C
ATOM   4314  OD1 ASP A 441     17.145  63.377 -25.479  1.00  0.00           O
ATOM   4315  OD2 ASP A 441     18.159  65.280 -25.093  1.00  0.00           Ol-
ATOM   4316  H   ASP A 441     14.387  66.406 -27.826  1.00  0.00           H
ATOM   4317  HA  ASP A 441     15.293  63.592 -27.431  1.00  0.00           H
ATOM   4318 1HB  ASP A 441     17.246  64.944 -27.880  1.00  0.00           H
ATOM   4319 2HB  ASP A 441     16.650  66.260 -26.842  1.00  0.00           H
ATOM   4320  N   SER A 442     13.718  63.755 -25.405  1.00  0.00           N
ATOM   4321  CA  SER A 442     12.900  63.753 -24.206  1.00  0.00           C
ATOM   4322  C   SER A 442     12.496  62.310 -23.892  1.00  0.00           C
ATOM   4323  O   SER A 442     12.218  61.535 -24.804  1.00  0.00           O
ATOM   4324  CB  SER A 442     11.648  64.628 -24.388  1.00  0.00           C
ATOM   4325  OG  SER A 442     11.959  65.952 -24.816  1.00  0.00           O
ATOM   4326  H   SER A 442     13.649  62.929 -25.983  1.00  0.00           H
ATOM   4327  HA  SER A 442     13.463  64.190 -23.381  1.00  0.00           H
ATOM   4328 1HB  SER A 442     10.996  64.179 -25.138  1.00  0.00           H
ATOM   4329 2HB  SER A 442     11.114  64.701 -23.441  1.00  0.00           H
ATOM   4330  HG  SER A 442     11.147  66.455 -24.915  1.00  0.00           H
ATOM   4331  N   LEU A 443     12.456  61.971 -22.607  1.00  0.00           N
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ATOM   4332  CA  LEU A 443      11.981  60.706 -22.064  1.00  0.00           C
ATOM   4333  C   LEU A 443      11.259  61.098 -20.778  1.00  0.00           C
ATOM   4334  O   LEU A 443      11.648  62.100 -20.171  1.00  0.00           O
ATOM   4335  CB  LEU A 443      13.158  59.771 -21.750  1.00  0.00           C
ATOM   4336  CG  LEU A 443      13.902  59.244 -22.988  1.00  0.00           C
ATOM   4337  CD1 LEU A 443      15.163  58.501 -22.531  1.00  0.00           C
ATOM   4338  CD2 LEU A 443      13.029  58.294 -23.818  1.00  0.00           C
ATOM   4339  H   LEU A 443      12.776  62.620 -21.903  1.00  0.00           H
ATOM   4340  HA  LEU A 443      11.291  60.244 -22.770  1.00  0.00           H
ATOM   4341  1HB LEU A 443      13.891  60.300 -21.141  1.00  0.00           H
ATOM   4342  2HB LEU A 443      12.795  58.899 -21.204  1.00  0.00           H
ATOM   4343  HG  LEU A 443      14.167  60.080 -23.635  1.00  0.00           H
ATOM   4344  1HD1 LEU A 443      15.698  58.124 -23.403  1.00  0.00           H
ATOM   4345  2HD1 LEU A 443      15.808  59.184 -21.978  1.00  0.00           H
ATOM   4346  3HD1 LEU A 443      14.882  57.667 -21.889  1.00  0.00           H
ATOM   4347  1HD2 LEU A 443      13.593  57.945 -24.683  1.00  0.00           H
ATOM   4348  2HD2 LEU A 443      12.738  57.440 -23.206  1.00  0.00           H
ATOM   4349  3HD2 LEU A 443      12.136  58.821 -24.155  1.00  0.00           H
ATOM   4350  N   THR A 444      10.223  60.361 -20.384  1.00  0.00           N
ATOM   4351  CA  THR A 444       9.065  60.983 -19.757  1.00  0.00           C
ATOM   4352  C   THR A 444       8.552  60.149 -18.575  1.00  0.00           C
ATOM   4353  O   THR A 444       8.595  58.921 -18.621  1.00  0.00           O
ATOM   4354  CB  THR A 444       8.005  61.135 -20.859  1.00  0.00           C
ATOM   4355  CG2 THR A 444       6.762  61.894 -20.391  1.00  0.00           C
ATOM   4356  OG1 THR A 444       8.572  61.817 -21.966  1.00  0.00           O
ATOM   4357  H   THR A 444      10.235  59.360 -20.518  1.00  0.00           H
ATOM   4358  HA  THR A 444       9.326  61.989 -19.428  1.00  0.00           H
ATOM   4359  HB  THR A 444       7.703  60.149 -21.212  1.00  0.00           H
ATOM   4360  1HG2 THR A 444       6.050  61.969 -21.213  1.00  0.00           H
ATOM   4361  2HG2 THR A 444       6.301  61.361 -19.559  1.00  0.00           H
ATOM   4362  3HG2 THR A 444       7.048  62.895 -20.066  1.00  0.00           H
ATOM   4363  HG1 THR A 444       7.911  61.914 -22.656  1.00  0.00           H
ATOM   4364  N   LEU A 445       8.060  60.800 -17.518  1.00  0.00           N
ATOM   4365  CA  LEU A 445       7.563  60.155 -16.309  1.00  0.00           C
ATOM   4366  C   LEU A 445       6.350  60.928 -15.797  1.00  0.00           C
ATOM   4367  O   LEU A 445       6.403  62.152 -15.703  1.00  0.00           O
ATOM   4368  CB  LEU A 445       8.679  60.166 -15.251  1.00  0.00           C
ATOM   4369  CG  LEU A 445       8.238  59.721 -13.843  1.00  0.00           C
ATOM   4370  CD1 LEU A 445       7.713  58.285 -13.833  1.00  0.00           C
ATOM   4371  CD2 LEU A 445       9.432  59.781 -12.889  1.00  0.00           C
ATOM   4372  H   LEU A 445       8.015  61.809 -17.523  1.00  0.00           H
ATOM   4373  HA  LEU A 445       7.273  59.129 -16.538  1.00  0.00           H
ATOM   4374  1HB LEU A 445       9.478  59.492 -15.558  1.00  0.00           H
ATOM   4375  2HB LEU A 445       9.075  61.177 -15.151  1.00  0.00           H
ATOM   4376  HG  LEU A 445       7.435  60.368 -13.491  1.00  0.00           H
ATOM   4377  1HD1 LEU A 445       7.414  58.014 -12.820  1.00  0.00           H
ATOM   4378  2HD1 LEU A 445       6.853  58.208 -14.498  1.00  0.00           H
ATOM   4379  3HD1 LEU A 445       8.497  57.609 -14.173  1.00  0.00           H
ATOM   4380  1HD2 LEU A 445       9.119  59.466 -11.894  1.00  0.00           H
ATOM   4381  2HD2 LEU A 445      10.219  59.119 -13.248  1.00  0.00           H
ATOM   4382  3HD2 LEU A 445       9.810  60.803 -12.844  1.00  0.00           H
ATOM   4383  N   VAL A 446       5.290  60.221 -15.409  1.00  0.00           N
ATOM   4384  CA  VAL A 446       4.163  60.798 -14.699  1.00  0.00           C
ATOM   4385  C   VAL A 446       4.340  60.480 -13.208  1.00  0.00           C
ATOM   4386  O   VAL A 446       4.668  59.346 -12.850  1.00  0.00           O
ATOM   4387  CB  VAL A 446       2.839  60.245 -15.253  1.00  0.00           C
ATOM   4388  CGI VAL A 446       1.645  60.969 -14.618  1.00  0.00           C
ATOM   4389  CG2 VAL A 446       2.755  60.392 -16.779  1.00  0.00           C
ATOM   4390  H   VAL A 446       5.244  59.232 -15.606  1.00  0.00           H
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ATOM   4391  HA  VAL A 446      4.118  61.869 -14.895   1.00  0.00           H
ATOM   4392  HB  VAL A 446      2.779  59.176 -15.053   1.00  0.00           H
ATOM   4393 1HG1 VAL A 446      0.717  60.565 -15.023   1.00  0.00           H
ATOM   4394 2HG1 VAL A 446      1.663  60.824 -13.538   1.00  0.00           H
ATOM   4395 3HG1 VAL A 446      1.704  62.034 -14.842   1.00  0.00           H
ATOM   4396 1HG2 VAL A 446      1.805  59.990 -17.132   1.00  0.00           H
ATOM   4397 2HG2 VAL A 446      2.825  61.445 -17.048   1.00  0.00           H
ATOM   4398 3HG2 VAL A 446      3.575  59.843 -17.243   1.00  0.00           H
ATOM   4399  N   PHE A 447      4.123  61.470 -12.344   1.00  0.00           N
ATOM   4400  CA  PHE A 447      4.295  61.357 -10.901   1.00  0.00           C
ATOM   4401  C   PHE A 447      2.914  61.436 -10.252   1.00  0.00           C
ATOM   4402  O   PHE A 447      2.200  62.413 -10.473   1.00  0.00           O
ATOM   4403  CB  PHE A 447      5.188  62.506 -10.397   1.00  0.00           C
ATOM   4404  CG  PHE A 447      6.470  62.065  -9.721   1.00  0.00           C
ATOM   4405  CD1 PHE A 447      6.471  61.706  -8.360   1.00  0.00           C
ATOM   4406  CD2 PHE A 447      7.682  62.020 -10.437   1.00  0.00           C
ATOM   4407  CE1 PHE A 447      7.665  61.336  -7.718   1.00  0.00           C
ATOM   4408  CE2 PHE A 447      8.877  61.639  -9.802   1.00  0.00           C
ATOM   4409  CZ  PHE A 447      8.870  61.296  -8.440   1.00  0.00           C
ATOM   4410  H   PHE A 447      3.817  62.373 -12.677   1.00  0.00           H
ATOM   4411  HA  PHE A 447      4.770  60.405 -10.665   1.00  0.00           H
ATOM   4412 1HB  PHE A 447      5.477  63.138 -11.236   1.00  0.00           H
ATOM   4413 2HB  PHE A 447      4.638  63.100  -9.667   1.00  0.00           H
ATOM   4414  HD1 PHE A 447      5.547  61.713  -7.800   1.00  0.00           H
ATOM   4415  HD2 PHE A 447      7.700  62.281 -11.485   1.00  0.00           H
ATOM   4416  HE1 PHE A 447      7.657  61.083  -6.668   1.00  0.00           H
ATOM   4417  HE2 PHE A 447      9.800  61.610 -10.362   1.00  0.00           H
ATOM   4418  HZ  PHE A 447      9.785  61.002  -7.948   1.00  0.00           H
ATOM   4419  N   VAL A 448      2.562  60.443  -9.439   1.00  0.00           N
ATOM   4420  CA  VAL A 448      1.281  60.345  -8.748   1.00  0.00           C
ATOM   4421  C   VAL A 448      1.549  60.052  -7.266   1.00  0.00           C
ATOM   4422  O   VAL A 448      2.687  59.784  -6.874   1.00  0.00           O
ATOM   4423  CB  VAL A 448      0.420  59.217  -9.374   1.00  0.00           C
ATOM   4424  CGI VAL A 448     -0.268  59.650 -10.667   1.00  0.00           C
ATOM   4425  CG2 VAL A 448      1.202  57.934  -9.670   1.00  0.00           C
ATOM   4426  H   VAL A 448      3.204  59.683  -9.263   1.00  0.00           H
ATOM   4427  HA  VAL A 448      0.734  61.281  -8.862   1.00  0.00           H
ATOM   4428  HB  VAL A 448     -0.321  58.880  -8.648   1.00  0.00           H
ATOM   4429 1HG1 VAL A 448     -0.857  58.821 -11.061   1.00  0.00           H
ATOM   4430 2HG1 VAL A 448     -0.924  60.496 -10.465   1.00  0.00           H
ATOM   4431 3HG1 VAL A 448      0.484  59.940 -11.400   1.00  0.00           H
ATOM   4432 1HG2 VAL A 448      0.532  57.192 -10.106   1.00  0.00           H
ATOM   4433 2HG2 VAL A 448      2.007  58.152 -10.372   1.00  0.00           H
ATOM   4434 3HG2 VAL A 448      1.623  57.542  -8.744   1.00  0.00           H
ATOM   4435  N   GLU A 449      0.492  60.018  -6.459   1.00  0.00           N
ATOM   4436  CA  GLU A 449      0.311  59.045  -5.392   1.00  0.00           C
ATOM   4437  C   GLU A 449     -1.149  58.545  -5.416   1.00  0.00           C
ATOM   4438  O   GLU A 449     -1.543  57.717  -4.595   1.00  0.00           O
ATOM   4439  CB  GLU A 449      0.749  59.636  -4.039   1.00  0.00           C
ATOM   4440  CG  GLU A 449      0.873  58.614  -2.889   1.00  0.00           C
ATOM   4441  CD  GLU A 449      1.811  57.463  -3.213   1.00  0.00           C
ATOM   4442  OE1 GLU A 449      2.921  57.746  -3.702   1.00  0.00           O
ATOM   4443  OE2 GLU A 449      1.423  56.294  -2.994   1.00  0.00           Ol-
ATOM   4444  H   GLU A 449     -0.248  60.697  -6.567   1.00  0.00           H
ATOM   4445  HA  GLU A 449      1.061  58.260  -5.484   1.00  0.00           H
ATOM   4446 1HB  GLU A 449      1.727  60.105  -4.146   1.00  0.00           H
ATOM   4447 2HB  GLU A 449      0.022  60.382  -3.716   1.00  0.00           H
ATOM   4448 1HG  GLU A 449      1.258  59.112  -1.999   1.00  0.00           H
ATOM   4449 2HG  GLU A 449     -0.107  58.189  -2.672   1.00  0.00           H
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ATOM   4450  N   THR A 450     -1.978  59.007  -6.359  1.00  0.00           N
ATOM   4451  CA  THR A 450     -3.322  58.492  -6.533  1.00  0.00           C
ATOM   4452  C   THR A 450     -3.259  56.972  -6.730  1.00  0.00           C
ATOM   4453  O   THR A 450     -2.750  56.472  -7.734  1.00  0.00           O
ATOM   4454  CB  THR A 450     -4.009  59.189  -7.720  1.00  0.00           C
ATOM   4455  CG2 THR A 450     -4.771  60.427  -7.257  1.00  0.00           C
ATOM   4456  OG1 THR A 450     -3.077  59.569  -8.713  1.00  0.00           O
ATOM   4457  H   THR A 450     -1.674  59.742  -6.982  1.00  0.00           H
ATOM   4458  HA  THR A 450     -3.931  58.767  -5.672  1.00  0.00           H
ATOM   4459  HB  THR A 450     -4.689  58.491  -8.207  1.00  0.00           H
ATOM   4460  1HG2 THR A 450     -5.248  60.902  -8.114  1.00  0.00           H
ATOM   4461  2HG2 THR A 450     -5.532  60.136  -6.533  1.00  0.00           H
ATOM   4462  3HG2 THR A 450     -4.078  61.129  -6.793  1.00  0.00           H
ATOM   4463  HGl  THR A 450     -3.537  60.000  -9.437  1.00  0.00           H
ATOM   4464  N   LYS A 451     -3.785  56.208  -5.771  1.00  0.00           N
ATOM   4465  CA  LYS A 451     -3.362  54.828  -5.607  1.00  0.00           C
ATOM   4466  C   LYS A 451     -3.864  53.919  -6.730  1.00  0.00           C
ATOM   4467  O   LYS A 451     -3.424  52.775  -6.829  1.00  0.00           O
ATOM   4468  CB  LYS A 451     -3.783  54.309  -4.219  1.00  0.00           C
ATOM   4469  CG  LYS A 451     -3.128  55.071  -3.049  1.00  0.00           C
ATOM   4470  CD  LYS A 451     -1.804  54.467  -2.552  1.00  0.00           C
ATOM   4471  CE  LYS A 451     -0.777  54.253  -3.671  1.00  0.00           C
ATOM   4472  NZ  LYS A 451      0.533  53.852  -3.146  1.00  0.00           N1+
ATOM   4473  H   LYS A 451     -4.484  56.589  -5.149  1.00  0.00           H
ATOM   4474  HA  LYS A 451     -2.278  54.789  -5.500  1.00  0.00           H
ATOM   4475  1HB  LYS A 451     -4.863  54.407  -4.107  1.00  0.00           H
ATOM   4476  2HB  LYS A 451     -3.501  53.261  -4.122  1.00  0.00           H
ATOM   4477  1HG  LYS A 451     -2.913  56.094  -3.356  1.00  0.00           H
ATOM   4478  2HG  LYS A 451     -3.808  55.083  -2.197  1.00  0.00           H
ATOM   4479  1HD  LYS A 451     -1.353  55.133  -1.817  1.00  0.00           H
ATOM   4480  2HD  LYS A 451     -1.995  53.497  -2.094  1.00  0.00           H
ATOM   4481  1HE  LYS A 451     -1.128  53.469  -4.342  1.00  0.00           H
ATOM   4482  2HE  LYS A 451     -0.650  55.179  -4.230  1.00  0.00           H
ATOM   4483  1HZ  LYS A 451      1.178  53.722  -3.913  1.00  0.00           H
ATOM   4484  2HZ  LYS A 451      0.884  54.571  -2.530  1.00  0.00           H
ATOM   4485  3HZ  LYS A 451      0.441  52.986  -2.634  1.00  0.00           H
ATOM   4486  N   LYS A 452     -4.782  54.405  -7.568  1.00  0.00           N
ATOM   4487  CA  LYS A 452     -5.131  53.768  -8.826  1.00  0.00           C
ATOM   4488  C   LYS A 452     -5.291  54.822  -9.924  1.00  0.00           C
ATOM   4489  O   LYS A 452     -5.910  54.556 -10.949  1.00  0.00           O
ATOM   4490  CB  LYS A 452     -6.375  52.865  -8.663  1.00  0.00           C
ATOM   4491  CG  LYS A 452     -6.146  51.618  -7.783  1.00  0.00           C
ATOM   4492  CD  LYS A 452     -5.234  50.608  -8.501  1.00  0.00           C
ATOM   4493  CE  LYS A 452     -4.471  49.642  -7.584  1.00  0.00           C
ATOM   4494  NZ  LYS A 452     -3.472  48.879  -8.363  1.00  0.00           N1+
ATOM   4495  H   LYS A 452     -5.273  55.257  -7.339  1.00  0.00           H
ATOM   4496  HA  LYS A 452     -4.400  52.993  -9.056  1.00  0.00           H
ATOM   4497  1HB  LYS A 452     -7.180  53.436  -8.201  1.00  0.00           H
ATOM   4498  2HB  LYS A 452     -6.696  52.509  -9.641  1.00  0.00           H
ATOM   4499  1HG  LYS A 452     -5.674  51.915  -6.846  1.00  0.00           H
ATOM   4500  2HG  LYS A 452     -7.103  51.141  -7.572  1.00  0.00           H
ATOM   4501  1HD  LYS A 452     -5.832  49.990  -9.170  1.00  0.00           H
ATOM   4502  2HD  LYS A 452     -4.481  51.145  -9.078  1.00  0.00           H
ATOM   4503  1HE  LYS A 452     -3.958  50.208  -6.806  1.00  0.00           H
ATOM   4504  2HE  LYS A 452     -5.172  48.946  -7.125  1.00  0.00           H
ATOM   4505  1HZ  LYS A 452     -2.977  48.247  -7.749  1.00  0.00           H
ATOM   4506  2HZ  LYS A 452     -3.940  48.349  -9.084  1.00  0.00           H
ATOM   4507  3HZ  LYS A 452     -2.816  49.518  -8.788  1.00  0.00           H
ATOM   4508  N   GLY A 453     -4.649  55.981  -9.744  1.00  0.00           N
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ATOM 4509 CA GLY A 453 -4.277 56.846 -10.861 1.00 0.00 C
ATOM 4510 C GLY A 453 -3.001 56.285 -11.500 1.00 0.00 C
ATOM 4511 O GLY A 453 -2.503 56.793 -12.497 1.00 0.00 O
ATOM 4512 H GLY A 453 -4.406 56.285 -8.812 1.00 0.00 H
ATOM 4513 1HA GLY A 453 -5.084 56.863 -11.593 1.00 0.00 H
ATOM 4514 2HA GLY A 453 -4.098 57.857 -10.495 1.00 0.00 H
ATOM 4515 N ALA A 454 -2.468 55.217 -10.901 1.00 0.00 N
ATOM 4516 CA ALA A 454 -1.509 54.327 -11.511 1.00 0.00 C
ATOM 4517 C ALA A 454 -2.253 53.488 -12.557 1.00 0.00 C
ATOM 4518 O ALA A 454 -2.229 53.813 -13.741 1.00 0.00 O
ATOM 4519 CB ALA A 454 -0.853 53.498 -10.401 1.00 0.00 C
ATOM 4520 H ALA A 454 -2.731 54.986 -9.954 1.00 0.00 H
ATOM 4521 HA ALA A 454 -0.688 54.908 -11.930 1.00 0.00 H
ATOM 4522 1HB ALA A 454 -0.123 52.817 -10.838 1.00 0.00 H
ATOM 4523 2HB ALA A 454 -0.351 54.164 -9.698 1.00 0.00 H
ATOM 4524 3HB ALA A 454 -1.616 52.924 -9.875 1.00 0.00 H
ATOM 4525 N ASP A 455 -2.925 52.421 -12.115 1.00 0.00 N
ATOM 4526 CA ASP A 455 -3.662 51.492 -12.959 1.00 0.00 C
ATOM 4527 C ASP A 455 -4.556 52.236 -13.952 1.00 0.00 C
ATOM 4528 O ASP A 455 -4.500 51.978 -15.153 1.00 0.00 O
ATOM 4529 CB ASP A 455 -4.538 50.562 -12.105 1.00 0.00 C
ATOM 4530 CG ASP A 455 -3.776 49.668 -11.148 1.00 0.00 C
ATOM 4531 OD1 ASP A 455 -2.746 50.106 -10.587 1.00 0.00 O
ATOM 4532 OD2 ASP A 455 -4.286 48.583 -10.803 1.00 0.00 Ol-
ATOM 4533 H ASP A 455 -2.945 52.210 -11.128 1.00 0.00 H
ATOM 4534 HA ASP A 455 -2.960 50.862 -13.506 1.00 0.00 H
ATOM 4535 1HB ASP A 455 -5.219 51.159 -11.499 1.00 0.00 H
ATOM 4536 2HB ASP A 455 -5.113 49.904 -12.756 1.00 0.00 H
ATOM 4537 N SER A 456 -5.399 53.152 -13.463 1.00 0.00 N
ATOM 4538 CA SER A 456 -6.357 53.853 -14.305 1.00 0.00 C
ATOM 4539 C SER A 456 -5.667 55.038 -14.989 1.00 0.00 C
ATOM 4540 O SER A 456 -6.150 56.172 -14.963 1.00 0.00 O
ATOM 4541 CB SER A 456 -7.593 54.271 -13.492 1.00 0.00 C
ATOM 4542 OG SER A 456 -8.716 54.478 -14.336 1.00 0.00 O
ATOM 4543 H SER A 456 -5.385 53.376 -12.478 1.00 0.00 H
ATOM 4544 HA SER A 456 -6.809 53.150 -15.004 1.00 0.00 H
ATOM 4545 1HB SER A 456 -7.838 53.488 -12.773 1.00 0.00 H
ATOM 4546 2HB SER A 456 -7.382 55.199 -12.960 1.00 0.00 H
ATOM 4547 HG SER A 456 -9.473 54.737 -13.805 1.00 0.00 H
ATOM 4548 N LEU A 457 -4.563 54.744 -15.663 1.00 0.00 N
ATOM 4549 CA LEU A 457 -3.757 55.662 -16.439 1.00 0.00 C
ATOM 4550 C LEU A 457 -2.752 54.798 -17.192 1.00 0.00 C
ATOM 4551 O LEU A 457 -2.489 55.031 -18.367 1.00 0.00 O
ATOM 4552 CB LEU A 457 -3.066 56.711 -15.554 1.00 0.00 C
ATOM 4553 CG LEU A 457 -2.551 57.921 -16.354 1.00 0.00 C
ATOM 4554 CD1 LEU A 457 -3.704 58.805 -16.851 1.00 0.00 C
ATOM 4555 CD2 LEU A 457 -1.645 58.771 -15.456 1.00 0.00 C
ATOM 4556 H LEU A 457 -4.209 53.798 -15.663 1.00 0.00 H
ATOM 4557 HA LEU A 457 -4.402 56.244 -17.099 1.00 0.00 H
ATOM 4558 1HB LEU A 457 -3.772 57.081 -14.810 1.00 0.00 H
ATOM 4559 2HB LEU A 457 -2.212 56.258 -15.051 1.00 0.00 H
ATOM 4560 HG LEU A 457 -1.991 57.571 -17.221 1.00 0.00 H
ATOM 4561 1HD1 LEU A 457 -3.301 59.648 -17.411 1.00 0.00 H
ATOM 4562 2HD1 LEU A 457 -4.358 58.219 -17.498 1.00 0.00 H
ATOM 4563 3HD1 LEU A 457 -4.274 59.174 -15.999 1.00 0.00 H
ATOM 4564 1HD2 LEU A 457 -1.278 59.629 -16.019 1.00 0.00 H
ATOM 4565 2HD2 LEU A 457 -2.212 59.119 -14.593 1.00 0.00 H
ATOM 4566 3HD2 LEU A 457 -0.801 58.171 -15.118 1.00 0.00 H
ATOM 4567 N GLU A 458 -2.269 53.731 -16.548 1.00 0.00 N

ATOM 4568 CA GLU A 458 -1.681 52.601 -17.249 1.00 0.00 C
ATOM 4569 C GLU A 458 -2.637 52.182 -18.371 1.00 0.00 C
ATOM 4570 O GLU A 458 -2.231 52.128 -19.527 1.00 0.00 O
ATOM 4571 CB GLU A 458 -1.390 51.457 -16.266 1.00 0.00 C
ATOM 4572 CG GLU A 458 -0.229 50.565 -16.735 1.00 0.00 C
ATOM 4573 CD GLU A 458 0.221 49.607 -15.646 1.00 0.00 C
ATOM 4574 OE1 GLU A 458 -0.527 49.465 -14.664 1.00 0.00 O
ATOM 4575 OE2 GLU A 458 1.375 49.127 -15.664 1.00 0.00 Ol-
ATOM 4576 H GLU A 458 -2.305 53.690 -15.539 1.00 0.00 H
ATOM 4577 HA GLU A 458 -0.691 52.874 -17.614 1.00 0.00 H
ATOM 4578 1HB GLU A 458 -1.124 51.871 -15.293 1.00 0.00 H
ATOM 4579 2HB GLU A 458 -2.276 50.831 -16.163 1.00 0.00 H
ATOM 4580 1HG GLU A 458 -0.548 49.977 -17.597 1.00 0.00 H
ATOM 4581 2HG GLU A 458 0.619 51.189 -17.015 1.00 0.00 H
ATOM 4582 N ASP A 459 -3.900 51.952 -17.994 1.00 0.00 N
ATOM 4583 CA ASP A 459 -5.090 51.924 -18.843 1.00 0.00 C
ATOM 4584 C ASP A 459 -4.945 52.833 -20.070 1.00 0.00 C
ATOM 4585 O ASP A 459 -4.784 52.364 -21.196 1.00 0.00 O
ATOM 4586 CB ASP A 459 -6.284 52.352 -17.967 1.00 0.00 C
ATOM 4587 CG ASP A 459 -7.476 52.870 -18.752 1.00 0.00 C
ATOM 4588 OD1 ASP A 459 -7.836 52.240 -19.761 1.00 0.00 O
ATOM 4589 OD2 ASP A 459 -8.001 53.926 -18.335 1.00 0.00 Ol-
ATOM 4590 H ASP A 459 -4.112 51.772 -17.023 1.00 0.00 H
ATOM 4591 HA ASP A 459 -5.287 50.900 -19.158 1.00 0.00 H
ATOM 4592 1HB ASP A 459 -6.631 51.499 -17.384 1.00 0.00 H
ATOM 4593 2HB ASP A 459 -5.973 53.150 -17.293 1.00 0.00 H
ATOM 4594 N PHE A 460 -5.040 54.142 -19.833 1.00 0.00 N
ATOM 4595 CA PHE A 460 -5.060 55.163 -20.867 1.00 0.00 C
ATOM 4596 C PHE A 460 -3.870 54.988 -21.807 1.00 0.00 C
ATOM 4597 O PHE A 460 -3.995 55.080 -23.022 1.00 0.00 O
ATOM 4598 CB PHE A 460 -5.011 56.534 -20.176 1.00 0.00 C
ATOM 4599 CG PHE A 460 -5.111 57.772 -21.049 1.00 0.00 C
ATOM 4600 CD1 PHE A 460 -6.027 57.849 -22.117 1.00 0.00 C
ATOM 4601 CD2 PHE A 460 -4.294 58.888 -20.776 1.00 0.00 C
ATOM 4602 CE1 PHE A 460 -6.132 59.023 -22.884 1.00 0.00 C
ATOM 4603 CE2 PHE A 460 -4.391 60.059 -21.548 1.00 0.00 C
ATOM 4604 CZ PHE A 460 -5.318 60.130 -22.598 1.00 0.00 C
ATOM 4605 H PHE A 460 -5.104 54.480 -18.884 1.00 0.00 H
ATOM 4606 HA PHE A 460 -5.991 55.092 -21.430 1.00 0.00 H
ATOM 4607 1HB PHE A 460 -5.839 56.617 -19.472 1.00 0.00 H
ATOM 4608 2HB PHE A 460 -4.068 56.639 -19.641 1.00 0.00 H
ATOM 4609 HD1 PHE A 460 -6.654 57.003 -22.353 1.00 0.00 H
ATOM 4610 HD2 PHE A 460 -3.581 58.851 -19.965 1.00 0.00 H
ATOM 4611 HE1 PHE A 460 -6.842 59.075 -23.697 1.00 0.00 H
ATOM 4612 HE2 PHE A 460 -3.751 60.902 -21.333 1.00 0.00 H
ATOM 4613 HZ PHE A 460 -5.408 61.033 -23.184 1.00 0.00 H
ATOM 4614 N LEU A 461 -2.699 54.749 -21.227 1.00 0.00 N
ATOM 4615 CA LEU A 461 -1.445 54.748 -21.956 1.00 0.00 C
ATOM 4616 C LEU A 461 -1.102 53.331 -22.422 1.00 0.00 C
ATOM 4617 O LEU A 461 0.032 53.041 -22.797 1.00 0.00 O
ATOM 4618 CB LEU A 461 -0.363 55.374 -21.067 1.00 0.00 C
ATOM 4619 CG LEU A 461 -0.762 56.755 -20.513 1.00 0.00 C
ATOM 4620 CD1 LEU A 461 0.343 57.265 -19.584 1.00 0.00 C
ATOM 4621 CD2 LEU A 461 -1.064 57.767 -21.623 1.00 0.00 C
ATOM 4622 H LEU A 461 -2.655 54.557 -20.236 1.00 0.00 H
ATOM 4623 HA LEU A 461 -1.502 55.462 -22.778 1.00 0.00 H
ATOM 4624 1HB LEU A 461 -0.168 54.721 -20.217 1.00 0.00 H
ATOM 4625 2HB LEU A 461 0.553 55.502 -21.645 1.00 0.00 H
ATOM 4626 HG LEU A 461 -1.730 56.683 -20.018 1.00 0.00 H

ATOM 4627 1HD1 LEU A 461 0.065 58.242 -19.190 1.00 0.00 H
ATOM 4628 2HD1 LEU A 461 0.477 56.565 -18.759 1.00 0.00 H
ATOM 4629 3HD1 LEU A 461 1.276 57.351 -20.142 1.00 0.00 H
ATOM 4630 1HD2 LEU A 461 -1.340 58.723 -21.178 1.00 0.00 H
ATOM 4631 2HD2 LEU A 461 -0.179 57.898 -22.246 1.00 0.00 H
ATOM 4632 3HD2 LEU A 461 -1.888 57.400 -22.235 1.00 0.00 H
ATOM 4633 N TYR A 462 -2.091 52.443 -22.400 1.00 0.00 N
ATOM 4634 CA TYR A 462 -2.044 51.114 -22.968 1.00 0.00 C
ATOM 4635 C TYR A 462 -3.052 51.114 -24.110 1.00 0.00 C
ATOM 4636 O TYR A 462 -2.687 50.852 -25.255 1.00 0.00 O
ATOM 4637 CB TYR A 462 -2.371 50.065 -21.894 1.00 0.00 C
ATOM 4638 CG TYR A 462 -2.837 48.728 -22.434 1.00 0.00 C
ATOM 4639 CD1 TYR A 462 -1.924 47.809 -22.982 1.00 0.00 C
ATOM 4640 CD2 TYR A 462 -4.203 48.392 -22.407 1.00 0.00 C
ATOM 4641 CE1 TYR A 462 -2.372 46.579 -23.497 1.00 0.00 C
ATOM 4642 CE2 TYR A 462 -4.652 47.167 -22.923 1.00 0.00 C
ATOM 4643 CZ TYR A 462 -3.739 46.248 -23.474 1.00 0.00 C
ATOM 4644 OH TYR A 462 -4.171 45.056 -23.981 1.00 0.00 O
ATOM 4645 H TYR A 462 -2.969 52.675 -21.959 1.00 0.00 H
ATOM 4646 HA TYR A 462 -1.029 50.895 -23.298 1.00 0.00 H
ATOM 4647 1HB TYR A 462 -1.483 49.869 -21.294 1.00 0.00 H
ATOM 4648 2HB TYR A 462 -3.168 50.439 -21.251 1.00 0.00 H
ATOM 4649 HD1 TYR A 462 -0.870 48.045 -23.009 1.00 0.00 H
ATOM 4650 HD2 TYR A 462 -4.920 49.080 -21.985 1.00 0.00 H
ATOM 4651 HE1 TYR A 462 -1.664 45.879 -23.915 1.00 0.00 H
ATOM 4652 HE2 TYR A 462 -5.704 46.924 -22.900 1.00 0.00 H
ATOM 4653 HH TYR A 462 -5.125 44.994 -23.885 1.00 0.00 H
ATOM 4654 N HIS A 463 -4.310 51.429 -23.798 1.00 0.00 N
ATOM 4655 CA HIS A 463 -5.386 51.479 -24.773 1.00 0.00 C
ATOM 4656 C HIS A 463 -5.042 52.449 -25.899 1.00 0.00 C
ATOM 4657 O HIS A 463 -5.084 52.062 -27.067 1.00 0.00 O
ATOM 4658 CB HIS A 463 -6.719 51.805 -24.088 1.00 0.00 C
ATOM 4659 CG HIS A 463 -7.237 50.637 -23.282 1.00 0.00 C
ATOM 4660 CD2 HIS A 463 -7.484 49.333 -23.636 1.00 0.00 C
ATOM 4661 ND1 HIS A 463 -7.565 50.709 -21.933 1.00 0.00 N
ATOM 4662 CE1 HIS A 463 -7.964 49.493 -21.533 1.00 0.00 C
ATOM 4663 NE2 HIS A 463 -7.926 48.613 -22.535 1.00 0.00 N
ATOM 4664 H HIS A 463 -4.553 51.648 -22.843 1.00 0.00 H
ATOM 4665 HA HIS A 463 -5.610 50.470 -25.119 1.00 0.00 H
ATOM 4666 1HB HIS A 463 -6.584 52.652 -23.414 1.00 0.00 H
ATOM 4667 2HB HIS A 463 -7.464 52.057 -24.842 1.00 0.00 H
ATOM 4668 HD2 HIS A 463 -7.325 49.010 -24.654 1.00 0.00 H
ATOM 4669 HD1 HIS A 463 -7.478 51.585 -21.438 1.00 0.00 H
ATOM 4670 HE1 HIS A 463 -8.262 49.332 -20.508 1.00 0.00 H
ATOM 4671 N GLU A 464 -4.618 53.668 -25.560 1.00 0.00 N
ATOM 4672 CA GLU A 464 -4.324 54.679 -26.562 1.00 0.00 C
ATOM 4673 C GLU A 464 -2.860 54.564 -27.017 1.00 0.00 C
ATOM 4674 O GLU A 464 -2.301 55.479 -27.617 1.00 0.00 O
ATOM 4675 CB GLU A 464 -4.662 56.074 -26.017 1.00 0.00 C
ATOM 4676 CG GLU A 464 -6.063 56.143 -25.386 1.00 0.00 C
ATOM 4677 CD GLU A 464 -7.140 55.619 -26.320 1.00 0.00 C
ATOM 4678 OE1 GLU A 464 -7.215 56.160 -27.443 1.00 0.00 O
ATOM 4679 OE2 GLU A 464 -7.860 54.693 -25.891 1.00 0.00 Ol-
ATOM 4680 H GLU A 464 -4.493 53.907 -24.586 1.00 0.00 H
ATOM 4681 HA GLU A 464 -5.032 54.591 -27.386 1.00 0.00 H
ATOM 4682 1HB GLU A 464 -3.938 56.351 -25.251 1.00 0.00 H
ATOM 4683 2HB GLU A 464 -4.627 56.800 -26.829 1.00 0.00 H
ATOM 4684 1HG GLU A 464 -6.083 55.543 -24.476 1.00 0.00 H
ATOM 4685 2HG GLU A 464 -6.302 57.179 -25.142 1.00 0.00 H

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ATOM   4686  N   GLY A 465     -2.206  53.434 -26.733  1.00  0.00           N
ATOM   4687  CA  GLY A 465     -1.033  53.008 -27.475  1.00  0.00           C
ATOM   4688  C   GLY A 465      0.279  53.604 -26.960  1.00  0.00           C
ATOM   4689  O   GLY A 465      1.353  53.215 -27.426  1.00  0.00           O
ATOM   4690  H   GLY A 465     -2.524  52.842 -25.979  1.00  0.00           H
ATOM   4691  1HA GLY A 465     -0.938  51.924 -27.415  1.00  0.00           H
ATOM   4692  2HA GLY A 465     -1.134  53.307 -28.518  1.00  0.00           H
ATOM   4693  N   TYR A 466      0.230  54.512 -25.984  1.00  0.00           N
ATOM   4694  CA  TYR A 466      1.402  55.229 -25.495  1.00  0.00           C
ATOM   4695  C   TYR A 466      2.226  54.356 -24.537  1.00  0.00           C
ATOM   4696  O   TYR A 466      2.428  54.725 -23.383  1.00  0.00           O
ATOM   4697  CB  TYR A 466      0.969  56.532 -24.809  1.00  0.00           C
ATOM   4698  CG  TYR A 466      0.240  57.520 -25.695  1.00  0.00           C
ATOM   4699  CD1 TYR A 466      0.947  58.289 -26.638  1.00  0.00           C
ATOM   4700  CD2 TYR A 466     -1.151  57.692 -25.586  1.00  0.00           C
ATOM   4701  CE1 TYR A 466      0.274  59.210 -27.458  1.00  0.00           C
ATOM   4702  CE2 TYR A 466     -1.826  58.611 -26.407  1.00  0.00           C
ATOM   4703  CZ  TYR A 466     -1.117  59.382 -27.349  1.00  0.00           C
ATOM   4704  OH  TYR A 466     -1.767  60.278 -28.150  1.00  0.00           O
ATOM   4705  H   TYR A 466     -0.652  54.732 -25.544  1.00  0.00           H
ATOM   4706  HA  TYR A 466      2.006  55.559 -26.341  1.00  0.00           H
ATOM   4707  1HB TYR A 466      0.295  56.302 -23.984  1.00  0.00           H
ATOM   4708  2HB TYR A 466      1.848  57.051 -24.426  1.00  0.00           H
ATOM   4709  HD1 TYR A 466      2.016  58.174 -26.735  1.00  0.00           H
ATOM   4710  HD2 TYR A 466     -1.712  57.115 -24.866  1.00  0.00           H
ATOM   4711  HE1 TYR A 466      0.825  59.793 -28.181  1.00  0.00           H
ATOM   4712  HE2 TYR A 466     -2.896  58.731 -26.319  1.00  0.00           H
ATOM   4713  HH  TYR A 466     -2.705  60.269 -27.946  1.00  0.00           H
ATOM   4714  N   ALA A 467      2.728  53.229 -25.058  1.00  0.00           N
ATOM   4715  CA  ALA A 467      3.366  52.121 -24.358  1.00  0.00           C
ATOM   4716  C   ALA A 467      4.007  52.505 -23.019  1.00  0.00           C
ATOM   4717  O   ALA A 467      4.943  53.305 -22.978  1.00  0.00           O
ATOM   4718  CB  ALA A 467      4.408  51.485 -25.281  1.00  0.00           C
ATOM   4719  H   ALA A 467      2.688  53.072 -26.055  1.00  0.00           H
ATOM   4720  HA  ALA A 467      2.641  51.321 -24.206  1.00  0.00           H
ATOM   4721  1HB ALA A 467      4.892  50.655 -24.766  1.00  0.00           H
ATOM   4722  2HB ALA A 467      3.920  51.118 -26.183  1.00  0.00           H
ATOM   4723  3HB ALA A 467      5.157  52.229 -25.551  1.00  0.00           H
ATOM   4724  N   CYS A 468      3.560  51.864 -21.938  1.00  0.00           N
ATOM   4725  CA  CYS A 468      3.615  52.423 -20.596  1.00  0.00           C
ATOM   4726  C   CYS A 468      3.917  51.334 -19.566  1.00  0.00           C
ATOM   4727  O   CYS A 468      4.158  50.178 -19.920  1.00  0.00           O
ATOM   4728  CB  CYS A 468      2.238  53.040 -20.294  1.00  0.00           C
ATOM   4729  SG  CYS A 468      0.984  51.726 -20.134  1.00  0.00           S
ATOM   4730  H   CYS A 468      3.158  50.942 -22.028  1.00  0.00           H
ATOM   4731  HA  CYS A 468      4.408  53.170 -20.545  1.00  0.00           H
ATOM   4732  1HB CYS A 468      2.288  53.602 -19.361  1.00  0.00           H
ATOM   4733  2HB CYS A 468      1.953  53.709 -21.106  1.00  0.00           H
ATOM   4734  HG  CYS A 468      0.004  52.178 -19.918  1.00  0.00           H
ATOM   4735  N   THR A 469      3.844  51.712 -18.294  1.00  0.00           N
ATOM   4736  CA  THR A 469      3.462  50.874 -17.171  1.00  0.00           C
ATOM   4737  C   THR A 469      3.290  51.835 -15.983  1.00  0.00           C
ATOM   4738  O   THR A 469      3.779  52.969 -16.040  1.00  0.00           O
ATOM   4739  CB  THR A 469      4.455  49.725 -16.905  1.00  0.00           C
ATOM   4740  CG2 THR A 469      5.917  50.182 -16.875  1.00  0.00           C
ATOM   4741  OG1 THR A 469      4.142  49.070 -15.688  1.00  0.00           O
ATOM   4742  H   THR A 469      4.066  52.663 -18.036  1.00  0.00           H
ATOM   4743  HA  THR A 469      2.581  50.289 -17.437  1.00  0.00           H
ATOM   4744  HB  THR A 469      4.323  48.948 -17.658  1.00  0.00           H
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ATOM 4745 1HG2 THR A 469 6.562 49.325 -16.683 1.00 0.00 H
ATOM 4746 2HG2 THR A 469 6.179 50.626 -17.835 1.00 0.00 H
ATOM 4747 3HG2 THR A 469 6.051 50.922 -16.085 1.00 0.00 H
ATOM 4748 HG1 THR A 469 4.769 48.359 -15.537 1.00 0.00 H
ATOM 4749 N SER A 470 2.613 51.412 -14.916 1.00 0.00 N
ATOM 4750 CA SER A 470 2.489 52.166 -13.690 1.00 0.00 C
ATOM 4751 C SER A 470 3.122 51.352 -12.561 1.00 0.00 C
ATOM 4752 O SER A 470 2.524 50.445 -11.981 1.00 0.00 O
ATOM 4753 CB SER A 470 1.035 52.597 -13.440 1.00 0.00 C
ATOM 4754 OG SER A 470 0.166 51.550 -13.051 1.00 0.00 O
ATOM 4755 H SER A 470 2.149 50.516 -14.934 1.00 0.00 H
ATOM 4756 HA SER A 470 2.888 53.169 -13.838 1.00 0.00 H
ATOM 4757 1HB SER A 470 1.008 53.340 -12.643 1.00 0.00 H
ATOM 4758 2HB SER A 470 0.621 53.027 -14.352 1.00 0.00 H
ATOM 4759 HG SER A 470 -0.717 51.901 -12.916 1.00 0.00 H
ATOM 4760 N ILE A 471 4.369 51.676 -12.228 1.00 0.00 N
ATOM 4761 CA ILE A 471 5.107 50.901 -11.256 1.00 0.00 C
ATOM 4762 C ILE A 471 4.841 51.577 -9.912 1.00 0.00 C
ATOM 4763 O ILE A 471 5.703 52.258 -9.351 1.00 0.00 O
ATOM 4764 CB ILE A 471 6.594 50.791 -11.649 1.00 0.00 C
ATOM 4765 CGI ILE A 471 6.733 50.293 -13.101 1.00 0.00 C
ATOM 4766 CG2 ILE A 471 7.298 49.790 -10.723 1.00 0.00 C
ATOM 4767 CD1 ILE A 471 8.194 50.177 -13.552 1.00 0.00 C
ATOM 4768 H ILE A 471 4.815 52.474 -12.657 1.00 0.00 H
ATOM 4769 HA ILE A 471 4.814 49.854 -11.327 1.00 0.00 H
ATOM 4770 HB ILE A 471 7.064 51.771 -11.573 1.00 0.00 H
ATOM 4771 1HG1 ILE A 471 6.278 49.307 -13.194 1.00 0.00 H
ATOM 4772 2HG1 ILE A 471 6.232 50.989 -13.774 1.00 0.00 H
ATOM 4773 1HG2 ILE A 471 8.348 49.712 -11.002 1.00 0.00 H
ATOM 4774 2HG2 ILE A 471 7.220 50.132 -9.691 1.00 0.00 H
ATOM 4775 3HG2 ILE A 471 6.824 48.812 -10.817 1.00 0.00 H
ATOM 4776 1HD1 ILE A 471 8.230 49.823 -14.582 1.00 0.00 H
ATOM 4777 2HD1 ILE A 471 8.673 51.154 -13.487 1.00 0.00 H
ATOM 4778 3HD1 ILE A 471 8.719 49.472 -12.907 1.00 0.00 H
ATOM 4779 N HIS A 472 3.628 51.388 -9.391 1.00 0.00 N
ATOM 4780 CA HIS A 472 3.264 51.944 -8.099 1.00 0.00 C
ATOM 4781 C HIS A 472 3.937 51.144 -6.977 1.00 0.00 C
ATOM 4782 O HIS A 472 4.408 50.024 -7.190 1.00 0.00 O
ATOM 4783 CB HIS A 472 1.750 52.157 -7.940 1.00 0.00 C
ATOM 4784 CG HIS A 472 0.832 50.964 -7.947 1.00 0.00 C
ATOM 4785 CD2 HIS A 472 0.121 50.344 -8.944 1.00 0.00 C
ATOM 4786 ND1 HIS A 472 0.479 50.298 -6.785 1.00 0.00 N
ATOM 4787 CE1 HIS A 472 -0.351 49.295 -7.107 1.00 0.00 C
ATOM 4788 NE2 HIS A 472 -0.614 49.287 -8.413 1.00 0.00 N
ATOM 4789 H HIS A 472 2.940 50.848 -9.896 1.00 0.00 H
ATOM 4790 HA HIS A 472 3.416 53.023 -8.111 1.00 0.00 H
ATOM 4791 1HB HIS A 472 1.549 52.646 -6.986 1.00 0.00 H
ATOM 4792 2HB HIS A 472 1.383 52.785 -8.753 1.00 0.00 H
ATOM 4793 HD2 HIS A 472 0.191 50.702 -9.960 1.00 0.00 H
ATOM 4794 HD1 HIS A 472 0.848 50.604 -5.895 1.00 0.00 H
ATOM 4795 HE1 HIS A 472 -0.714 48.626 -6.341 1.00 0.00 H
ATOM 4796 N GLY A 473 4.107 51.749 -5.802 1.00 0.00 N
ATOM 4797 CA GLY A 473 4.813 51.157 -4.672 1.00 0.00 C
ATOM 4798 C GLY A 473 4.172 49.851 -4.221 1.00 0.00 C
ATOM 4799 O GLY A 473 4.828 49.010 -3.615 1.00 0.00 O
ATOM 4800 H GLY A 473 3.735 52.677 -5.654 1.00 0.00 H
ATOM 4801 1HA GLY A 473 5.845 50.950 -4.956 1.00 0.00 H
ATOM 4802 2HA GLY A 473 4.800 51.851 -3.831 1.00 0.00 H
ATOM 4803 N ASP A 474 2.889 49.717 -4.527 1.00 0.00 N

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ATOM   4804  CA  ASP A 474      1.987  48.697  -4.034  1.00  0.00           C
ATOM   4805  C   ASP A 474      1.796  47.640  -5.135  1.00  0.00           C
ATOM   4806  O   ASP A 474      0.888  46.814  -5.068  1.00  0.00           O
ATOM   4807  CB  ASP A 474      0.650  49.341  -3.581  1.00  0.00           C
ATOM   4808  CG  ASP A 474      0.660  50.861  -3.438  1.00  0.00           C
ATOM   4809  OD1 ASP A 474      0.964  51.546  -4.445  1.00  0.00           O
ATOM   4810  OD2 ASP A 474      0.358  51.376  -2.344  1.00  0.00           Ol-
ATOM   4811  H   ASP A 474      2.451  50.368  -5.163  1.00  0.00           H
ATOM   4812  HA  ASP A 474      2.379  48.281  -3.106  1.00  0.00           H
ATOM   4813 1HB  ASP A 474     -0.130  49.109  -4.306  1.00  0.00           H
ATOM   4814 2HB  ASP A 474      0.367  48.945  -2.606  1.00  0.00           H
ATOM   4815  N   ARG A 475      2.637  47.681  -6.174  1.00  0.00           N
ATOM   4816  CA  ARG A 475      2.785  46.584  -7.124  1.00  0.00           C
ATOM   4817  C   ARG A 475      3.590  45.475  -6.443  1.00  0.00           C
ATOM   4818  O   ARG A 475      4.359  45.734  -5.517  1.00  0.00           O
ATOM   4819  CB  ARG A 475      3.502  47.062  -8.397  1.00  0.00           C
ATOM   4820  CG  ARG A 475      2.610  47.917  -9.301  1.00  0.00           C
ATOM   4821  CD  ARG A 475      1.688  47.071 -10.199  1.00  0.00           C
ATOM   4822  NE  ARG A 475      0.550  47.873 -10.681  1.00  0.00           N
ATOM   4823  CZ  ARG A 475      0.258  48.272 -11.930  1.00  0.00           C
ATOM   4824  NH1 ARG A 475      1.048  47.975 -12.962  1.00  0.00           N1+
ATOM   4825  NH2 ARG A 475     -0.852  48.965 -12.135  1.00  0.00           N
ATOM   4826  H   ARG A 475      3.208  48.499  -6.330  1.00  0.00           H
ATOM   4827  HA  ARG A 475      1.800  46.226  -7.422  1.00  0.00           H
ATOM   4828 1HB  ARG A 475      4.368  47.665  -8.122  1.00  0.00           H
ATOM   4829 2HB  ARG A 475      3.830  46.199  -8.976  1.00  0.00           H
ATOM   4830 1HG  ARG A 475      1.980  48.560  -8.688  1.00  0.00           H
ATOM   4831 2HG  ARG A 475      3.234  48.532  -9.950  1.00  0.00           H
ATOM   4832 1HD  ARG A 475      2.251  46.707 -11.059  1.00  0.00           H
ATOM   4833 2HD  ARG A 475      1.305  46.223  -9.631  1.00  0.00           H
ATOM   4834  HE  ARG A 475     -0.058  48.126  -9.915  1.00  0.00           H
ATOM   4835 1HH1 ARG A 475      0.804  48.288 -13.891  1.00  0.00           H
ATOM   4836 2HH1 ARG A 475      1.890  47.437 -12.815  1.00  0.00           H
ATOM   4837 1HH2 ARG A 475     -1.090  49.274 -13.066  1.00  0.00           H
ATOM   4838 2HH2 ARG A 475     -1.461  49.184 -11.359  1.00  0.00           H
ATOM   4839  N   SER A 476      3.431  44.229  -6.883  1.00  0.00           N
ATOM   4840  CA  SER A 476      3.995  43.116  -6.154  1.00  0.00           C
ATOM   4841  C   SER A 476      5.525  43.084  -6.260  1.00  0.00           C
ATOM   4842  O   SER A 476      6.128  43.551  -7.230  1.00  0.00           O
ATOM   4843  CB  SER A 476      3.358  41.795  -6.612  1.00  0.00           C
ATOM   4844  OG  SER A 476      3.563  41.548  -7.990  1.00  0.00           O
ATOM   4845  H   SER A 476      2.914  44.057  -7.734  1.00  0.00           H
ATOM   4846  HA  SER A 476      3.647  43.144  -5.121  1.00  0.00           H
ATOM   4847 1HB  SER A 476      3.794  40.967  -6.053  1.00  0.00           H
ATOM   4848 2HB  SER A 476      2.283  41.827  -6.432  1.00  0.00           H
ATOM   4849  HG  SER A 476      3.151  40.716  -8.232  1.00  0.00           H
ATOM   4850  N   GLN A 477      6.152  42.443  -5.273  1.00  0.00           N
ATOM   4851  CA  GLN A 477      7.557  42.080  -5.292  1.00  0.00           C
ATOM   4852  C   GLN A 477      7.710  40.933  -6.302  1.00  0.00           C
ATOM   4853  O   GLN A 477      7.962  39.789  -5.929  1.00  0.00           O
ATOM   4854  CB  GLN A 477      7.937  41.740  -3.836  1.00  0.00           C
ATOM   4855  CG  GLN A 477      9.285  41.060  -3.580  1.00  0.00           C
ATOM   4856  CD  GLN A 477     10.422  41.656  -4.389  1.00  0.00           C
ATOM   4857  NE2 GLN A 477     10.700  41.058  -5.534  1.00  0.00           N
ATOM   4858  OE1 GLN A 477     11.043  42.629  -3.976  1.00  0.00           O
ATOM   4859  H   GLN A 477      5.644  42.177  -4.442  1.00  0.00           H
ATOM   4860  HA  GLN A 477      8.157  42.960  -5.525  1.00  0.00           H
ATOM   4861 1HB  GLN A 477      7.967  42.655  -3.244  1.00  0.00           H
ATOM   4862 2HB  GLN A 477      7.195  41.060  -3.416  1.00  0.00           H
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ATOM 4863 1HG GLN A 477 9.547 41.157 -2.526 1.00 0.00 H
ATOM 4864 2HG GLN A 477 9.215 40.004 -3.840 1.00 0.00 H
ATOM 4865 1HE2 GLN A 477 11.446 41.408 -6.117 1.00 0.00 H
ATOM 4866 2HE2 GLN A 477 10.167 40.252 -5.825 1.00 0.00 H
ATOM 4867 N ARG A 478 7.553 41.265 -7.583 1.00 0.00 N
ATOM 4868 CA ARG A 478 7.415 40.394 -8.740 1.00 0.00 C
ATOM 4869 C ARG A 478 7.160 41.342 -9.919 1.00 0.00 C
ATOM 4870 O ARG A 478 8.015 41.495 -10.789 1.00 0.00 O
ATOM 4871 CB ARG A 478 6.270 39.381 -8.544 1.00 0.00 C
ATOM 4872 CG ARG A 478 6.285 38.240 -9.571 1.00 0.00 C
ATOM 4873 CD ARG A 478 4.950 38.108 -10.316 1.00 0.00 C
ATOM 4874 NE ARG A 478 4.865 39.085 -11.409 1.00 0.00 N
ATOM 4875 CZ ARG A 478 4.031 40.121 -11.552 1.00 0.00 C
ATOM 4876 NH1 ARG A 478 3.187 40.457 -10.580 1.00 0.00 N1+
ATOM 4877 NH2 ARG A 478 4.042 40.838 -12.664 1.00 0.00 N
ATOM 4878 H ARG A 478 7.517 42.238 -7.852 1.00 0.00 H
ATOM 4879 HA ARG A 478 8.321 39.799 -8.858 1.00 0.00 H
ATOM 4880 1HB ARG A 478 6.347 38.932 -7.554 1.00 0.00 H
ATOM 4881 2HB ARG A 478 5.312 39.892 -8.637 1.00 0.00 H
ATOM 4882 1HG ARG A 478 7.066 38.425 -10.309 1.00 0.00 H
ATOM 4883 2HG ARG A 478 6.482 37.296 -9.063 1.00 0.00 H
ATOM 4884 1HD ARG A 478 4.864 37.105 -10.734 1.00 0.00 H
ATOM 4885 2HD ARG A 478 4.127 38.284 -9.623 1.00 0.00 H
ATOM 4886 HE ARG A 478 5.559 38.894 -12.118 1.00 0.00 H
ATOM 4887 1HH1 ARG A 478 2.562 41.242 -10.702 1.00 0.00 H
ATOM 4888 2HH1 ARG A 478 3.170 39.929 -9.719 1.00 0.00 H
ATOM 4889 1HH2 ARG A 478 3.411 41.620 -12.768 1.00 0.00 H
ATOM 4890 2HH2 ARG A 478 4.683 40.605 -13.409 1.00 0.00 H
ATOM 4891 N ASP A 479 6.039 42.081 -9.882 1.00 0.00 N
ATOM 4892 CA ASP A 479 5.794 43.196 -10.798 1.00 0.00 C
ATOM 4893 C ASP A 479 7.025 44.089 -10.821 1.00 0.00 C
ATOM 4894 O ASP A 479 7.519 44.475 -11.876 1.00 0.00 O
ATOM 4895 CB ASP A 479 4.650 44.100 -10.318 1.00 0.00 C
ATOM 4896 CG ASP A 479 3.263 43.517 -10.419 1.00 0.00 C
ATOM 4897 OD1 ASP A 479 2.937 42.938 -11.473 1.00 0.00 O
ATOM 4898 OD2 ASP A 479 2.558 43.571 -9.390 1.00 0.00 Ol-
ATOM 4899 H ASP A 479 5.322 41.875 -9.201 1.00 0.00 H
ATOM 4900 HA ASP A 479 5.669 42.814 -11.811 1.00 0.00 H
ATOM 4901 1HB ASP A 479 4.798 44.347 -9.267 1.00 0.00 H
ATOM 4902 2HB ASP A 479 4.638 45.016 -10.908 1.00 0.00 H
ATOM 4903 N ARG A 480 7.502 44.445 -9.628 1.00 0.00 N
ATOM 4904 CA ARG A 480 8.583 45.398 -9.471 1.00 0.00 C
ATOM 4905 C ARG A 480 9.943 44.694 -9.519 1.00 0.00 C
ATOM 4906 O ARG A 480 10.929 45.220 -9.007 1.00 0.00 O
ATOM 4907 CB ARG A 480 8.343 46.236 -8.204 1.00 0.00 C
ATOM 4908 CG ARG A 480 9.062 47.593 -8.275 1.00 0.00 C
ATOM 4909 CD ARG A 480 8.380 48.643 -7.387 1.00 0.00 C
ATOM 4910 NE ARG A 480 8.938 49.981 -7.657 1.00 0.00 N
ATOM 4911 CZ ARG A 480 8.286 51.151 -7.622 1.00 0.00 C
ATOM 4912 NH1 ARG A 480 7.002 51.210 -7.286 1.00 0.00 N1+
ATOM 4913 NH2 ARG A 480 8.939 52.257 -7.949 1.00 0.00 N
ATOM 4914 H ARG A 480 7.109 44.046 -8.788 1.00 0.00 H
ATOM 4915 HA ARG A 480 8.467 46.202 -10.198 1.00 0.00 H
ATOM 4916 1HB ARG A 480 7.276 46.420 -8.086 1.00 0.00 H
ATOM 4917 2HB ARG A 480 8.717 45.696 -7.335 1.00 0.00 H
ATOM 4918 1HG ARG A 480 10.092 47.478 -7.939 1.00 0.00 H
ATOM 4919 2HG ARG A 480 9.054 47.957 -9.303 1.00 0.00 H
ATOM 4920 1HD ARG A 480 7.310 48.655 -7.594 1.00 0.00 H
ATOM 4921 2HD ARG A 480 8.544 48.394 -6.338 1.00 0.00 H

ATOM 4922 HE ARG A 480 9.921 49.957 -7.888 1.00 0.00 H
ATOM 4923 1HH1 ARG A 480 6.526 52.100 -7.265 1.00 0.00 H
ATOM 4924 2HH1 ARG A 480 6.501 50.364 -7.052 1.00 0.00 H
ATOM 4925 1HH2 ARG A 480 8.465 53.148 -7.929 1.00 0.00 H
ATOM 4926 2HH2 ARG A 480 9.911 52.209 -8.219 1.00 0.00 H
ATOM 4927 N GLU A 481 9.990 43.533 -10.175 1.00 0.00 N
ATOM 4928 CA GLU A 481 11.181 42.975 -10.783 1.00 0.00 C
ATOM 4929 C GLU A 481 10.985 43.161 -12.290 1.00 0.00 C
ATOM 4930 O GLU A 481 11.717 43.901 -12.947 1.00 0.00 O
ATOM 4931 CB GLU A 481 11.322 41.480 -10.440 1.00 0.00 C
ATOM 4932 CG GLU A 481 11.422 41.200 -8.936 1.00 0.00 C
ATOM 4933 CD GLU A 481 12.712 41.713 -8.336 1.00 0.00 C
ATOM 4934 OE1 GLU A 481 13.656 42.047 -9.079 1.00 0.00 O
ATOM 4935 OE2 GLU A 481 12.784 41.773 -7.094 1.00 0.00 Ol-
ATOM 4936 H GLU A 481 9.153 42.976 -10.275 1.00 0.00 H
ATOM 4937 HA GLU A 481 12.058 43.521 -10.433 1.00 0.00 H
ATOM 4938 1HB GLU A 481 10.454 40.938 -10.814 1.00 0.00 H
ATOM 4939 2HB GLU A 481 12.225 41.084 -10.904 1.00 0.00 H
ATOM 4940 1HG GLU A 481 10.594 41.687 -8.419 1.00 0.00 H
ATOM 4941 2HG GLU A 481 11.375 40.125 -8.762 1.00 0.00 H
ATOM 4942 N GLU A 482 9.966 42.489 -12.826 1.00 0.00 N
ATOM 4943 CA GLU A 482 9.666 42.401 -14.242 1.00 0.00 C
ATOM 4944 C GLU A 482 9.595 43.790 -14.886 1.00 0.00 C
ATOM 4945 O GLU A 482 10.270 44.064 -15.880 1.00 0.00 O
ATOM 4946 CB GLU A 482 8.346 41.641 -14.397 1.00 0.00 C
ATOM 4947 CG GLU A 482 8.473 40.178 -13.935 1.00 0.00 C
ATOM 4948 CD GLU A 482 7.116 39.560 -13.660 1.00 0.00 C
ATOM 4949 OE1 GLU A 482 6.106 40.112 -14.140 1.00 0.00 O
ATOM 4950 OE2 GLU A 482 7.068 38.570 -12.903 1.00 0.00 Ol-
ATOM 4951 H GLU A 482 9.326 41.984 -12.230 1.00 0.00 H
ATOM 4952 HA GLU A 482 10.418 41.786 -14.736 1.00 0.00 H
ATOM 4953 1HB GLU A 482 7.575 42.124 -13.797 1.00 0.00 H
ATOM 4954 2HB GLU A 482 8.045 41.644 -15.445 1.00 0.00 H
ATOM 4955 1HG GLU A 482 8.967 39.593 -14.711 1.00 0.00 H
ATOM 4956 2HG GLU A 482 9.063 40.136 -13.019 1.00 0.00 H
ATOM 4957 N ALA A 483 8.767 44.671 -14.327 1.00 0.00 N
ATOM 4958 CA ALA A 483 8.459 45.955 -14.931 1.00 0.00 C
ATOM 4959 C ALA A 483 9.678 46.881 -14.910 1.00 0.00 C
ATOM 4960 O ALA A 483 9.719 47.876 -15.635 1.00 0.00 O
ATOM 4961 CB ALA A 483 7.267 46.599 -14.222 1.00 0.00 C
ATOM 4962 H ALA A 483 8.323 44.459 -13.446 1.00 0.00 H
ATOM 4963 HA ALA A 483 8.094 45.802 -15.946 1.00 0.00 H
ATOM 4964 1HB ALA A 483 7.045 47.561 -14.683 1.00 0.00 H
ATOM 4965 2HB ALA A 483 6.397 45.947 -14.307 1.00 0.00 H
ATOM 4966 3HB ALA A 483 7.507 46.748 -13.169 1.00 0.00 H
ATOM 4967 N LEU A 484 10.694 46.580 -14.095 1.00 0.00 N
ATOM 4968 CA LEU A 484 11.932 47.339 -14.148 1.00 0.00 C
ATOM 4969 C LEU A 484 12.574 47.152 -15.523 1.00 0.00 C
ATOM 4970 O LEU A 484 13.263 48.045 -16.014 1.00 0.00 O
ATOM 4971 CB LEU A 484 12.912 46.921 -13.042 1.00 0.00 C
ATOM 4972 CG LEU A 484 12.352 47.018 -11.612 1.00 0.00 C
ATOM 4973 CD1 LEU A 484 13.433 46.552 -10.630 1.00 0.00 C
ATOM 4974 CD2 LEU A 484 11.932 48.448 -11.249 1.00 0.00 C
ATOM 4975 H LEU A 484 10.605 45.820 -13.436 1.00 0.00 H
ATOM 4976 HA LEU A 484 11.725 48.389 -13.942 1.00 0.00 H
ATOM 4977 1HB LEU A 484 13.209 45.883 -13.192 1.00 0.00 H
ATOM 4978 2HB LEU A 484 13.794 47.560 -13.076 1.00 0.00 H
ATOM 4979 HG LEU A 484 11.466 46.389 -11.525 1.00 0.00 H
ATOM 4980 1HD1 LEU A 484 13.051 46.615 -9.611 1.00 0.00 H

ATOM 4981 2HD1 LEU A 484 13.707 45.521 -10.852 1.00 0.00 H
ATOM 4982 3HD1 LEU A 484 14.312 47.189 -10.727 1.00 0.00 H
ATOM 4983 1HD2 LEU A 484 11.543 48.465 -10.231 1.00 0.00 H
ATOM 4984 2HD2 LEU A 484 12.795 49.109 -11.320 1.00 0.00 H
ATOM 4985 3HD2 LEU A 484 11.158 48.786 -11.939 1.00 0.00 H
ATOM 4986 N HIS A 485 12.340 45.998 -16.151 1.00 0.00 N
ATOM 4987 CA HIS A 485 12.907 45.673 -17.446 1.00 0.00 C
ATOM 4988 C HIS A 485 12.048 46.269 -18.569 1.00 0.00 C
ATOM 4989 O HIS A 485 12.329 46.056 -19.749 1.00 0.00 O
ATOM 4990 CB HIS A 485 13.086 44.153 -17.585 1.00 0.00 C
ATOM 4991 CG HIS A 485 14.187 43.750 -18.539 1.00 0.00 C
ATOM 4992 CD2 HIS A 485 15.061 42.690 -18.539 1.00 0.00 C
ATOM 4993 ND1 HIS A 485 14.517 44.489 -19.670 1.00 0.00 N
ATOM 4994 CE1 HIS A 485 15.544 43.881 -20.284 1.00 0.00 C
ATOM 4995 NE2 HIS A 485 15.911 42.784 -19.631 1.00 0.00 N
ATOM 4996 H HIS A 485 11.744 45.303 -15.724 1.00 0.00 H
ATOM 4997 HA HIS A 485 13.945 46.004 -17.482 1.00 0.00 H
ATOM 4998 1HB HIS A 485 13.329 43.725 -16.612 1.00 0.00 H
ATOM 4999 2HB HIS A 485 12.161 43.710 -17.955 1.00 0.00 H
ATOM 5000 HD2 HIS A 485 15.008 41.948 -17.756 1.00 0.00 H
ATOM 5001 HD1 HIS A 485 14.000 45.327 -19.894 1.00 0.00 H
ATOM 5002 HE1 HIS A 485 15.957 44.301 -21.189 1.00 0.00 H
ATOM 5003 N GLN A 486 11.019 47.049 -18.232 1.00 0.00 N
ATOM 5004 CA GLN A 486 10.378 47.916 -19.198 1.00 0.00 C
ATOM 5005 C GLN A 486 11.178 49.221 -19.242 1.00 0.00 C
ATOM 5006 O GLN A 486 12.275 49.263 -19.805 1.00 0.00 O
ATOM 5007 CB GLN A 486 8.889 48.120 -18.888 1.00 0.00 C
ATOM 5008 CG GLN A 486 8.072 46.856 -19.152 1.00 0.00 C
ATOM 5009 CD GLN A 486 6.599 47.132 -18.891 1.00 0.00 C
ATOM 5010 NE2 GLN A 486 5.984 47.961 -19.725 1.00 0.00 N
ATOM 5011 OE1 GLN A 486 6.039 46.637 -17.923 1.00 0.00 O
ATOM 5012 H GLN A 486 10.671 47.044 -17.284 1.00 0.00 H
ATOM 5013 HA GLN A 486 10.296 47.398 -20.154 1.00 0.00 H
ATOM 5014 1HB GLN A 486 8.770 48.390 -17.839 1.00 0.00 H
ATOM 5015 2HB GLN A 486 8.493 48.919 -19.515 1.00 0.00 H
ATOM 5016 1HG GLN A 486 8.202 46.548 -20.190 1.00 0.00 H
ATOM 5017 2HG GLN A 486 8.412 46.058 -18.492 1.00 0.00 H
ATOM 5018 1HE2 GLN A 486 5.006 48.176 -19.593 1.00 0.00 H
ATOM 5019 2HE2 GLN A 486 6.493 48.377 -20.491 1.00 0.00 H
ATOM 5020 N PHE A 487 10.618 50.280 -18.655 1.00 0.00 N
ATOM 5021 CA PHE A 487 11.095 51.648 -18.744 1.00 0.00 C
ATOM 5022 C PHE A 487 12.585 51.745 -18.438 1.00 0.00 C
ATOM 5023 O PHE A 487 13.343 52.346 -19.195 1.00 0.00 O
ATOM 5024 CB PHE A 487 10.274 52.510 -17.783 1.00 0.00 C
ATOM 5025 CG PHE A 487 10.577 53.991 -17.843 1.00 0.00 C
ATOM 5026 CD1 PHE A 487 9.947 54.795 -18.810 1.00 0.00 C
ATOM 5027 CD2 PHE A 487 11.452 54.593 -16.918 1.00 0.00 C
ATOM 5028 CE1 PHE A 487 10.143 56.183 -18.814 1.00 0.00 C
ATOM 5029 CE2 PHE A 487 11.654 55.984 -16.924 1.00 0.00 C
ATOM 5030 CZ PHE A 487 10.982 56.780 -17.866 1.00 0.00 C
ATOM 5031 H PHE A 487 9.789 50.165 -18.089 1.00 0.00 H
ATOM 5032 HA PHE A 487 10.879 52.044 -19.737 1.00 0.00 H
ATOM 5033 1HB PHE A 487 9.213 52.398 -18.008 1.00 0.00 H
ATOM 5034 2HB PHE A 487 10.463 52.193 -16.757 1.00 0.00 H
ATOM 5035 HD1 PHE A 487 9.309 54.344 -19.555 1.00 0.00 H
ATOM 5036 HD2 PHE A 487 11.976 53.985 -16.195 1.00 0.00 H
ATOM 5037 HE1 PHE A 487 9.645 56.796 -19.552 1.00 0.00 H
ATOM 5038 HE2 PHE A 487 12.323 56.436 -16.207 1.00 0.00 H
ATOM 5039 HZ PHE A 487 11.112 57.852 -17.858 1.00 0.00 H

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ATOM   5040  N   ARG A 488      13.026  51.130 -17.341  1.00  0.00           N
ATOM   5041  CA  ARG A 488      14.405  51.264 -16.901  1.00  0.00           C
ATOM   5042  C   ARG A 488      15.334  50.305 -17.656  1.00  0.00           C
ATOM   5043  O   ARG A 488      16.439  50.025 -17.199  1.00  0.00           O
ATOM   5044  CB  ARG A 488      14.514  51.137 -15.374  1.00  0.00           C
ATOM   5045  CG  ARG A 488      13.686  52.209 -14.646  1.00  0.00           C
ATOM   5046  CD  ARG A 488      14.056  52.225 -13.158  1.00  0.00           C
ATOM   5047  NE  ARG A 488      13.337  53.266 -12.392  1.00  0.00           N
ATOM   5048  CZ  ARG A 488      12.541  53.021 -11.338  1.00  0.00           C
ATOM   5049  NH1 ARG A 488      11.914  51.850 -11.244  1.00  0.00           N1+
ATOM   5050  NH2 ARG A 488      12.424  53.929 -10.375  1.00  0.00           N
ATOM   5051  H   ARG A 488      12.398  50.555 -16.797  1.00  0.00           H
ATOM   5052  HA  ARG A 488      14.704  52.311 -16.955  1.00  0.00           H
ATOM   5053  1HB ARG A 488      14.150  50.157 -15.064  1.00  0.00           H
ATOM   5054  2HB ARG A 488      15.556  51.249 -15.073  1.00  0.00           H
ATOM   5055  1HG ARG A 488      13.894  53.187 -15.080  1.00  0.00           H
ATOM   5056  2HG ARG A 488      12.625  51.984 -14.751  1.00  0.00           H
ATOM   5057  1HD ARG A 488      13.812  51.261 -12.712  1.00  0.00           H
ATOM   5058  2HD ARG A 488      15.124  52.416 -13.051  1.00  0.00           H
ATOM   5059  HE  ARG A 488      13.476  54.215 -12.710  1.00  0.00           H
ATOM   5060  1HH1 ARG A 488      11.314  51.661 -10.454  1.00  0.00           H
ATOM   5061  2HH1 ARG A 488      12.037  51.152 -11.963  1.00  0.00           H
ATOM   5062  1HH2 ARG A 488      11.826  53.748  -9.582  1.00  0.00           H
ATOM   5063  2HH2 ARG A 488      12.932  54.799 -10.437  1.00  0.00           H
ATOM   5064  N   SER A 489      14.938  49.844 -18.844  1.00  0.00           N
ATOM   5065  CA  SER A 489      15.883  49.359 -19.831  1.00  0.00           C
ATOM   5066  C   SER A 489      15.525  49.928 -21.209  1.00  0.00           C
ATOM   5067  O   SER A 489      15.951  49.383 -22.228  1.00  0.00           O
ATOM   5068  CB  SER A 489      15.860  47.826 -19.836  1.00  0.00           C
ATOM   5069  OG  SER A 489      14.617  47.345 -20.327  1.00  0.00           O
ATOM   5070  H   SER A 489      13.955  49.826 -19.077  1.00  0.00           H
ATOM   5071  HA  SER A 489      16.894  49.644 -19.539  1.00  0.00           H
ATOM   5072  1HB SER A 489      16.659  47.452 -20.476  1.00  0.00           H
ATOM   5073  2HB SER A 489      16.004  47.457 -18.821  1.00  0.00           H
ATOM   5074  HG  SER A 489      14.621  46.385 -20.323  1.00  0.00           H
ATOM   5075  N   GLY A 490      14.677  50.959 -21.246  1.00  0.00           N
ATOM   5076  CA  GLY A 490      14.101  51.519 -22.456  1.00  0.00           C
ATOM   5077  C   GLY A 490      13.215  50.486 -23.156  1.00  0.00           C
ATOM   5078  O   GLY A 490      13.717  49.620 -23.873  1.00  0.00           O
ATOM   5079  H   GLY A 490      14.391  51.409 -20.388  1.00  0.00           H
ATOM   5080  1HA GLY A 490      13.497  52.390 -22.202  1.00  0.00           H
ATOM   5081  2HA GLY A 490      14.900  51.818 -23.134  1.00  0.00           H
ATOM   5082  N   LYS A 491      11.899  50.570 -22.963  1.00  0.00           N
ATOM   5083  CA  LYS A 491      10.905  49.807 -23.708  1.00  0.00           C
ATOM   5084  C   LYS A 491       9.733  50.767 -23.884  1.00  0.00           C
ATOM   5085  O   LYS A 491       9.784  51.618 -24.766  1.00  0.00           O
ATOM   5086  CB  LYS A 491      10.517  48.494 -22.993  1.00  0.00           C
ATOM   5087  CG  LYS A 491      11.677  47.523 -22.722  1.00  0.00           C
ATOM   5088  CD  LYS A 491      12.290  46.927 -24.001  1.00  0.00           C
ATOM   5089  CE  LYS A 491      13.647  46.264 -23.723  1.00  0.00           C
ATOM   5090  NZ  LYS A 491      14.601  47.203 -23.099  1.00  0.00           N1+
ATOM   5091  H   LYS A 491      11.530  51.194 -22.260  1.00  0.00           H
ATOM   5092  HA  LYS A 491      11.343  49.452 -24.641  1.00  0.00           H
ATOM   5093  1HB LYS A 491      10.076  48.725 -22.023  1.00  0.00           H
ATOM   5094  2HB LYS A 491       9.794  47.949 -23.599  1.00  0.00           H
ATOM   5095  1HG LYS A 491      12.473  48.045 -22.192  1.00  0.00           H
ATOM   5096  2HG LYS A 491      11.320  46.691 -22.114  1.00  0.00           H
ATOM   5097  1HD LYS A 491      11.617  46.174 -24.411  1.00  0.00           H
ATOM   5098  2HD LYS A 491      12.439  47.719 -24.735  1.00  0.00           H
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ATOM   5099 1HE  LYS A 491     13.507  45.420 -23.047  1.00  0.00           H
ATOM   5100 2HE  LYS A 491     14.078  45.911 -24.660  1.00  0.00           H
ATOM   5101 1HZ  LYS A 491     15.479  46.732 -22.932  1.00  0.00           H
ATOM   5102 2HZ  LYS A 491     14.754  47.988 -23.717  1.00  0.00           H
ATOM   5103 3HZ  LYS A 491     14.225  47.534 -22.222  1.00  0.00           H
ATOM   5104 N    SER A 492      8.742  50.710 -22.996  1.00  0.00           N
ATOM   5105 CA   SER A 492      7.901  51.852 -22.700  1.00  0.00           C
ATOM   5106 C    SER A 492      8.810  53.078 -22.490  1.00  0.00           C
ATOM   5107 O    SER A 492      9.715  52.993 -21.658  1.00  0.00           O
ATOM   5108 CB   SER A 492      7.163  51.525 -21.390  1.00  0.00           C
ATOM   5109 OG   SER A 492      6.715  50.171 -21.362  1.00  0.00           O
ATOM   5110 H    SER A 492      8.555  49.849 -22.501  1.00  0.00           H
ATOM   5111 HA   SER A 492      7.247  52.052 -23.548  1.00  0.00           H
ATOM   5112 1HB  SER A 492      7.834  51.682 -20.545  1.00  0.00           H
ATOM   5113 2HB  SER A 492      6.294  52.175 -21.290  1.00  0.00           H
ATOM   5114 HG   SER A 492      6.260  50.000 -20.534  1.00  0.00           H
ATOM   5115 N    PRO A 493      8.609  54.206 -23.184  1.00  0.00           N
ATOM   5116 CA   PRO A 493      9.433  55.396 -23.002  1.00  0.00           C
ATOM   5117 C    PRO A 493      8.709  56.375 -22.066  1.00  0.00           C
ATOM   5118 O    PRO A 493      9.104  57.533 -21.920  1.00  0.00           O
ATOM   5119 CB   PRO A 493      9.598  55.962 -24.412  1.00  0.00           C
ATOM   5120 CG   PRO A 493      8.254  55.636 -25.067  1.00  0.00           C
ATOM   5121 CD   PRO A 493      7.852  54.304 -24.427  1.00  0.00           C
ATOM   5122 HA   PRO A 493     10.391  55.112 -22.566  1.00  0.00           H
ATOM   5123 1HB  PRO A 493      9.788  57.034 -24.354  1.00  0.00           H
ATOM   5124 2HB  PRO A 493     10.436  55.472 -24.906  1.00  0.00           H
ATOM   5125 1HG  PRO A 493      7.540  56.430 -24.849  1.00  0.00           H
ATOM   5126 2HG  PRO A 493      8.385  55.552 -26.146  1.00  0.00           H
ATOM   5127 1HD  PRO A 493      8.107  53.465 -25.074  1.00  0.00           H
ATOM   5128 2HD  PRO A 493      6.785  54.281 -24.206  1.00  0.00           H
ATOM   5129 N    ILE A 494      7.650  55.869 -21.433  1.00  0.00           N
ATOM   5130 CA   ILE A 494      6.713  56.548 -20.560  1.00  0.00           C
ATOM   5131 C    ILE A 494      6.493  55.599 -19.376  1.00  0.00           C
ATOM   5132 O    ILE A 494      6.607  54.378 -19.522  1.00  0.00           O
ATOM   5133 CB   ILE A 494      5.402  56.825 -21.330  1.00  0.00           C
ATOM   5134 CGI  ILE A 494      5.639  57.841 -22.466  1.00  0.00           C
ATOM   5135 CG2  ILE A 494      4.309  57.353 -20.387  1.00  0.00           C
ATOM   5136 CD1  ILE A 494      4.507  57.863 -23.498  1.00  0.00           C
ATOM   5137 H    ILE A 494      7.420  54.891 -21.536  1.00  0.00           H
ATOM   5138 HA   ILE A 494      7.134  57.502 -20.245  1.00  0.00           H
ATOM   5139 HB   ILE A 494      5.010  55.891 -21.730  1.00  0.00           H
ATOM   5140 1HG1 ILE A 494      5.722  58.843 -22.047  1.00  0.00           H
ATOM   5141 2HG1 ILE A 494      6.560  57.589 -22.993  1.00  0.00           H
ATOM   5142 1HG2 ILE A 494      3.398  57.540 -20.956  1.00  0.00           H
ATOM   5143 2HG2 ILE A 494      4.108  56.613 -19.613  1.00  0.00           H
ATOM   5144 3HG2 ILE A 494      4.645  58.281 -19.924  1.00  0.00           H
ATOM   5145 1HD1 ILE A 494      4.734  58.598 -24.271  1.00  0.00           H
ATOM   5146 2HD1 ILE A 494      4.409  56.877 -23.953  1.00  0.00           H
ATOM   5147 3HD1 ILE A 494      3.572  58.131 -23.007  1.00  0.00           H
ATOM   5148 N    LEU A 495      6.205  56.153 -18.202  1.00  0.00           N
ATOM   5149 CA   LEU A 495      6.095  55.440 -16.942  1.00  0.00           C
ATOM   5150 C    LEU A 495      5.222  56.300 -16.032  1.00  0.00           C
ATOM   5151 O    LEU A 495      5.254  57.525 -16.142  1.00  0.00           O
ATOM   5152 CB   LEU A 495      7.511  55.253 -16.364  1.00  0.00           C
ATOM   5153 CG   LEU A 495      7.605  54.813 -14.891  1.00  0.00           C
ATOM   5154 CD1  LEU A 495      7.022  53.419 -14.662  1.00  0.00           C
ATOM   5155 CD2  LEU A 495      9.072  54.768 -14.445  1.00  0.00           C
ATOM   5156 H    LEU A 495      6.042  57.148 -18.140  1.00  0.00           H
ATOM   5157 HA   LEU A 495      5.642  54.463 -17.115  1.00  0.00           H
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ATOM   5158 1HB  LEU A 495      8.039  54.488 -16.934  1.00  0.00           H
ATOM   5159 2HB  LEU A 495      8.056  56.194 -16.427  1.00  0.00           H
ATOM   5160  HG  LEU A 495      7.043  55.509 -14.267  1.00  0.00           H
ATOM   5161 1HD1 LEU A 495      7.112  53.156 -13.608  1.00  0.00           H
ATOM   5162 2HD1 LEU A 495      5.971  53.412 -14.949  1.00  0.00           H
ATOM   5163 3HD1 LEU A 495      7.568  52.693 -15.265  1.00  0.00           H
ATOM   5164 1HD2 LEU A 495      9.126  54.456 -13.402  1.00  0.00           H
ATOM   5165 2HD2 LEU A 495      9.619  54.057 -15.065  1.00  0.00           H
ATOM   5166 3HD2 LEU A 495      9.515  55.758 -14.551  1.00  0.00           H
ATOM   5167  N   VAL A 496      4.473  55.669 -15.131  1.00  0.00           N
ATOM   5168  CA  VAL A 496      3.740  56.328 -14.062  1.00  0.00           C
ATOM   5169  C   VAL A 496      4.296  55.760 -12.748  1.00  0.00           C
ATOM   5170  O   VAL A 496      4.567  54.557 -12.672  1.00  0.00           O
ATOM   5171  CB  VAL A 496      2.230  56.061 -14.227  1.00  0.00           C
ATOM   5172  CGI VAL A 496      1.408  56.878 -13.225  1.00  0.00           C
ATOM   5173  CG2 VAL A 496      1.727  56.326 -15.655  1.00  0.00           C
ATOM   5174  H   VAL A 496      4.386  54.663 -15.162  1.00  0.00           H
ATOM   5175  HA  VAL A 496      3.874  57.407 -14.140  1.00  0.00           H
ATOM   5176  HB  VAL A 496      2.037  54.992 -14.133  1.00  0.00           H
ATOM   5177 1HG1 VAL A 496      0.348  56.668 -13.367  1.00  0.00           H
ATOM   5178 2HG1 VAL A 496      1.698  56.608 -12.210  1.00  0.00           H
ATOM   5179 3HG1 VAL A 496      1.591  57.941 -13.385  1.00  0.00           H
ATOM   5180 1HG2 VAL A 496      0.658  56.121 -15.709  1.00  0.00           H
ATOM   5181 2HG2 VAL A 496      1.910  57.369 -15.917  1.00  0.00           H
ATOM   5182 3HG2 VAL A 496      2.257  55.679 -16.354  1.00  0.00           H
ATOM   5183  N   ALA A 497      4.501  56.585 -11.718  1.00  0.00           N
ATOM   5184  CA  ALA A 497      5.113  56.142 -10.471  1.00  0.00           C
ATOM   5185  C   ALA A 497      4.557  56.913  -9.275  1.00  0.00           C
ATOM   5186  O   ALA A 497      4.336  58.119  -9.358  1.00  0.00           O
ATOM   5187  CB  ALA A 497      6.630  56.326 -10.544  1.00  0.00           C
ATOM   5188  H   ALA A 497      4.230  57.555 -11.787  1.00  0.00           H
ATOM   5189  HA  ALA A 497      4.937  55.074 -10.338  1.00  0.00           H
ATOM   5190 1HB  ALA A 497      7.083  55.994  -9.610  1.00  0.00           H
ATOM   5191 2HB  ALA A 497      7.029  55.737 -11.371  1.00  0.00           H
ATOM   5192 3HB  ALA A 497      6.862  57.379 -10.705  1.00  0.00           H
ATOM   5193  N   THR A 498      4.358  56.207  -8.163  1.00  0.00           N
ATOM   5194  CA  THR A 498      3.839  56.762  -6.927  1.00  0.00           C
ATOM   5195  C   THR A 498      5.010  57.258  -6.078  1.00  0.00           C
ATOM   5196  O   THR A 498      5.941  56.480  -5.849  1.00  0.00           O
ATOM   5197  CB  THR A 498      3.076  55.646  -6.205  1.00  0.00           C
ATOM   5198  CG2 THR A 498      1.724  55.377  -6.872  1.00  0.00           C
ATOM   5199  OG1 THR A 498      3.875  54.474  -6.202  1.00  0.00           O
ATOM   5200  H   THR A 498      4.573  55.221  -8.145  1.00  0.00           H
ATOM   5201  HA  THR A 498      3.169  57.592  -7.154  1.00  0.00           H
ATOM   5202  HB  THR A 498      2.934  55.919  -5.160  1.00  0.00           H
ATOM   5203 1HG2 THR A 498      1.206  54.581  -6.338  1.00  0.00           H
ATOM   5204 2HG2 THR A 498      1.119  56.284  -6.847  1.00  0.00           H
ATOM   5205 3HG2 THR A 498      1.883  55.076  -7.908  1.00  0.00           H
ATOM   5206  HG1 THR A 498      3.405  53.768  -5.752  1.00  0.00           H
ATOM   5207  N   ALA A 499      4.954  58.508  -5.617  1.00  0.00           N
ATOM   5208  CA  ALA A 499      5.856  59.125  -4.655  1.00  0.00           C
ATOM   5209  C   ALA A 499      6.407  58.140  -3.618  1.00  0.00           C
ATOM   5210  O   ALA A 499      7.618  58.097  -3.370  1.00  0.00           O
ATOM   5211  CB  ALA A 499      5.132  60.281  -3.963  1.00  0.00           C
ATOM   5212  H   ALA A 499      4.227  59.132  -5.938  1.00  0.00           H
ATOM   5213  HA  ALA A 499      6.676  59.611  -5.185  1.00  0.00           H
ATOM   5214 1HB  ALA A 499      5.801  60.749  -3.241  1.00  0.00           H
ATOM   5215 2HB  ALA A 499      4.828  61.017  -4.707  1.00  0.00           H
ATOM   5216 3HB  ALA A 499      4.250  59.900  -3.447  1.00  0.00           H
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ATOM   5217  N   VAL A 500      5.525  57.358  -2.993  1.00  0.00           N
ATOM   5218  CA  VAL A 500      5.854  56.450  -1.904  1.00  0.00           C
ATOM   5219  C   VAL A 500      6.912  55.425  -2.335  1.00  0.00           C
ATOM   5220  O   VAL A 500      7.544  54.779  -1.503  1.00  0.00           O
ATOM   5221  CB  VAL A 500      4.574  55.792  -1.354  1.00  0.00           C
ATOM   5222  CGI VAL A 500      4.048  54.683  -2.274  1.00  0.00           C
ATOM   5223  CG2 VAL A 500      4.787  55.227   0.057  1.00  0.00           C
ATOM   5224  H   VAL A 500      4.553  57.371  -3.270  1.00  0.00           H
ATOM   5225  HA  VAL A 500      6.147  57.027  -1.027  1.00  0.00           H
ATOM   5226  HB  VAL A 500      3.812  56.555  -1.194  1.00  0.00           H
ATOM   5227 1HG1 VAL A 500      3.145  54.250  -1.842  1.00  0.00           H
ATOM   5228 2HG1 VAL A 500      3.817  55.102  -3.253  1.00  0.00           H
ATOM   5229 3HG1 VAL A 500      4.806  53.908  -2.380  1.00  0.00           H
ATOM   5230 1HG2 VAL A 500      3.862  54.771   0.410  1.00  0.00           H
ATOM   5231 2HG2 VAL A 500      5.576  54.476   0.033  1.00  0.00           H
ATOM   5232 3HG2 VAL A 500      5.075  56.034   0.732  1.00  0.00           H
ATOM   5233  N   ALA A 501      7.106  55.258  -3.642  1.00  0.00           N
ATOM   5234  CA  ALA A 501      8.159  54.451  -4.208  1.00  0.00           C
ATOM   5235  C   ALA A 501      8.665  55.141  -5.472  1.00  0.00           C
ATOM   5236  O   ALA A 501      8.765  54.521  -6.533  1.00  0.00           O
ATOM   5237  CB  ALA A 501      7.632  53.045  -4.486  1.00  0.00           C
ATOM   5238  H   ALA A 501      6.494  55.712  -4.306  1.00  0.00           H
ATOM   5239  HA  ALA A 501      8.948  54.312  -3.469  1.00  0.00           H
ATOM   5240 1HB  ALA A 501      8.428  52.436  -4.914  1.00  0.00           H
ATOM   5241 2HB  ALA A 501      7.290  52.594  -3.554  1.00  0.00           H
ATOM   5242 3HB  ALA A 501      6.800  53.100  -5.189  1.00  0.00           H
ATOM   5243  N   ALA A 502      9.007  56.422  -5.342  1.00  0.00           N
ATOM   5244  CA  ALA A 502      9.738  57.177  -6.347  1.00  0.00           C
ATOM   5245  C   ALA A 502     10.956  57.853  -5.708  1.00  0.00           C
ATOM   5246  O   ALA A 502     11.690  58.578  -6.377  1.00  0.00           O
ATOM   5247  CB  ALA A 502      8.815  58.195  -7.007  1.00  0.00           C
ATOM   5248  H   ALA A 502      8.757  56.929  -4.505  1.00  0.00           H
ATOM   5249  HA  ALA A 502     10.024  56.514  -7.164  1.00  0.00           H
ATOM   5250 1HB  ALA A 502      9.370  58.757  -7.759  1.00  0.00           H
ATOM   5251 2HB  ALA A 502      7.983  57.677  -7.484  1.00  0.00           H
ATOM   5252 3HB  ALA A 502      8.430  58.881  -6.253  1.00  0.00           H
ATOM   5253  N   ARG A 503     11.181  57.585  -4.421  1.00  0.00           N
ATOM   5254  CA  ARG A 503     12.491  57.676  -3.801  1.00  0.00           C
ATOM   5255  C   ARG A 503     13.014  56.249  -3.966  1.00  0.00           C
ATOM   5256  O   ARG A 503     12.482  55.326  -3.350  1.00  0.00           O
ATOM   5257  CB  ARG A 503     12.353  58.124  -2.329  1.00  0.00           C
ATOM   5258  CG  ARG A 503     11.600  59.464  -2.260  1.00  0.00           C
ATOM   5259  CD  ARG A 503     11.704  60.241  -0.937  1.00  0.00           C
ATOM   5260  NE  ARG A 503     10.518  61.107  -0.721  1.00  0.00           N
ATOM   5261  CZ  ARG A 503     10.081  61.576   0.465  1.00  0.00           C
ATOM   5262  NH1 ARG A 503     10.816  61.416   1.555  1.00  0.00           N1+
ATOM   5263  NH2 ARG A 503      8.889  62.158   0.573  1.00  0.00           N
ATOM   5264  H   ARG A 503     10.417  57.303  -3.823  1.00  0.00           H
ATOM   5265  HA  ARG A 503     13.086  58.431  -4.315  1.00  0.00           H
ATOM   5266 1HB  ARG A 503     11.799  57.370  -1.769  1.00  0.00           H
ATOM   5267 2HB  ARG A 503     13.344  58.245  -1.891  1.00  0.00           H
ATOM   5268 1HG  ARG A 503     11.980  60.135  -3.030  1.00  0.00           H
ATOM   5269 2HG  ARG A 503     10.536  59.292  -2.421  1.00  0.00           H
ATOM   5270 1HD  ARG A 503     11.773  59.538  -0.107  1.00  0.00           H
ATOM   5271 2HD  ARG A 503     12.593  60.871  -0.955  1.00  0.00           H
ATOM   5272  HE  ARG A 503     10.024  61.342  -1.570  1.00  0.00           H
ATOM   5273 1HH1 ARG A 503     10.486  61.768   2.442  1.00  0.00           H
ATOM   5274 2HH1 ARG A 503     11.706  60.943   1.499  1.00  0.00           H
ATOM   5275 1HH2 ARG A 503      8.576  62.504   1.469  1.00  0.00           H
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ATOM 5276 2HH2 ARG A 503 8.298 62.255 -0.240 1.00 0.00 H
ATOM 5277 N GLY A 504 13.930 56.017 -4.906 1.00 0.00 N
ATOM 5278 CA GLY A 504 14.085 54.688 -5.471 1.00 0.00 C
ATOM 5279 C GLY A 504 15.131 54.655 -6.582 1.00 0.00 C
ATOM 5280 O GLY A 504 16.243 55.148 -6.406 1.00 0.00 O
ATOM 5281 H GLY A 504 14.523 56.768 -5.231 1.00 0.00 H
ATOM 5282 1HA GLY A 504 14.397 53.995 -4.690 1.00 0.00 H
ATOM 5283 2HA GLY A 504 13.134 54.357 -5.890 1.00 0.00 H
ATOM 5284 N LEU A 505 14.798 54.060 -7.728 1.00 0.00 N
ATOM 5285 CA LEU A 505 15.719 53.986 -8.851 1.00 0.00 C
ATOM 5286 C LEU A 505 15.597 55.300 -9.611 1.00 0.00 C
ATOM 5287 O LEU A 505 14.571 55.548 -10.254 1.00 0.00 O
ATOM 5288 CB LEU A 505 15.414 52.777 -9.757 1.00 0.00 C
ATOM 5289 CG LEU A 505 16.459 51.657 -9.655 1.00 0.00 C
ATOM 5290 CD1 LEU A 505 15.844 50.306 -10.042 1.00 0.00 C
ATOM 5291 CD2 LEU A 505 17.631 51.957 -10.598 1.00 0.00 C
ATOM 5292 H LEU A 505 13.884 53.644 -7.835 1.00 0.00 H
ATOM 5293 HA LEU A 505 16.729 53.809 -8.481 1.00 0.00 H
ATOM 5294 1HB LEU A 505 14.450 52.350 -9.482 1.00 0.00 H
ATOM 5295 2HB LEU A 505 15.384 53.101 -10.797 1.00 0.00 H
ATOM 5296 HG LEU A 505 16.829 51.596 -8.631 1.00 0.00 H
ATOM 5297 1HD1 LEU A 505 16.601 49.526 -9.963 1.00 0.00 H
ATOM 5298 2HD1 LEU A 505 15.016 50.078 -9.371 1.00 0.00 H
ATOM 5299 3HD1 LEU A 505 15.478 50.354 -11.067 1.00 0.00 H
ATOM 5300 1HD2 LEU A 505 18.371 51.160 -10.524 1.00 0.00 H
ATOM 5301 2HD2 LEU A 505 17.266 52.018 -11.623 1.00 0.00 H
ATOM 5302 3HD2 LEU A 505 18.089 52.905 -10.318 1.00 0.00 H
ATOM 5303 N ASP A 506 16.649 56.110 -9.536 1.00 0.00 N
ATOM 5304 CA ASP A 506 16.773 57.356 -10.267 1.00 0.00 C
ATOM 5305 C ASP A 506 16.659 57.073 -11.768 1.00 0.00 C
ATOM 5306 O ASP A 506 16.782 55.936 -12.229 1.00 0.00 O
ATOM 5307 CB ASP A 506 18.094 58.042 -9.890 1.00 0.00 C
ATOM 5308 CG ASP A 506 18.215 59.491 -10.334 1.00 0.00 C
ATOM 5309 OD1 ASP A 506 19.222 60.127 -9.973 1.00 0.00 O
ATOM 5310 OD2 ASP A 506 17.320 60.033 -11.017 1.00 0.00 Ol-
ATOM 5311 H ASP A 506 17.429 55.871 -8.940 1.00 0.00 H
ATOM 5312 HA ASP A 506 16.022 58.062 -9.912 1.00 0.00 H
ATOM 5313 1HB ASP A 506 18.210 58.037 -8.806 1.00 0.00 H
ATOM 5314 2HB ASP A 506 18.926 57.505 -10.346 1.00 0.00 H
ATOM 5315 N ILE A 507 16.372 58.120 -12.522 1.00 0.00 N
ATOM 5316 CA ILE A 507 15.978 58.094 -13.909 1.00 0.00 C
ATOM 5317 C ILE A 507 16.858 59.059 -14.704 1.00 0.00 C
ATOM 5318 O ILE A 507 17.087 58.823 -15.887 1.00 0.00 O
ATOM 5319 CB ILE A 507 14.483 58.445 -14.000 1.00 0.00 C
ATOM 5320 CGI ILE A 507 14.206 59.860 -13.451 1.00 0.00 C
ATOM 5321 CG2 ILE A 507 13.644 57.388 -13.264 1.00 0.00 C
ATOM 5322 CD1 ILE A 507 12.718 60.203 -13.419 1.00 0.00 C
ATOM 5323 H ILE A 507 16.419 59.051 -12.133 1.00 0.00 H
ATOM 5324 HA ILE A 507 16.043 57.073 -14.286 1.00 0.00 H
ATOM 5325 HB ILE A 507 14.147 58.342 -15.032 1.00 0.00 H
ATOM 5326 1HG1 ILE A 507 14.587 59.936 -12.433 1.00 0.00 H
ATOM 5327 2HG1 ILE A 507 14.704 60.598 -14.080 1.00 0.00 H
ATOM 5328 1HG2 ILE A 507 12.588 57.647 -13.335 1.00 0.00 H
ATOM 5329 2HG2 ILE A 507 13.810 56.411 -13.718 1.00 0.00 H
ATOM 5330 3HG2 ILE A 507 13.940 57.354 -12.215 1.00 0.00 H
ATOM 5331 1HD1 ILE A 507 12.585 61.211 -13.023 1.00 0.00 H
ATOM 5332 2HD1 ILE A 507 12.311 60.154 -14.429 1.00 0.00 H
ATOM 5333 3HD1 ILE A 507 12.194 59.492 -12.781 1.00 0.00 H
ATOM 5334 N SER A 508 17.358 60.120 -14.059 1.00 0.00 N

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ATOM   5335  CA  SER A 508      18.363  61.038 -14.579  1.00  0.00           C
ATOM   5336  C   SER A 508      18.024  61.725 -15.915  1.00  0.00           C
ATOM   5337  O   SER A 508      17.802  62.937 -15.955  1.00  0.00           O
ATOM   5338  CB  SER A 508      19.724  60.337 -14.579  1.00  0.00           C
ATOM   5339  OG  SER A 508      20.046  59.964 -13.251  1.00  0.00           O
ATOM   5340  H   SER A 508      17.038  60.342 -13.127  1.00  0.00           H
ATOM   5341  HA  SER A 508      18.654  61.740 -13.797  1.00  0.00           H
ATOM   5342 1HB  SER A 508      19.676  59.450 -15.210  1.00  0.00           H
ATOM   5343 2HB  SER A 508      20.483  61.017 -14.966  1.00  0.00           H
ATOM   5344  HG  SER A 508      20.899  59.523 -13.240  1.00  0.00           H
ATOM   5345  N   ASN A 509      18.055  60.975 -17.016  1.00  0.00           N
ATOM   5346  CA  ASN A 509      17.932  61.459 -18.388  1.00  0.00           C
ATOM   5347  C   ASN A 509      16.466  61.433 -18.827  1.00  0.00           C
ATOM   5348  O   ASN A 509      16.152  61.579 -20.005  1.00  0.00           O
ATOM   5349  CB  ASN A 509      18.799  60.590 -19.310  1.00  0.00           C
ATOM   5350  CG  ASN A 509      18.809  61.076 -20.761  1.00  0.00           C
ATOM   5351  ND2 ASN A 509      18.703  60.161 -21.721  1.00  0.00           N
ATOM   5352  OD1 ASN A 509      18.930  62.266 -21.042  1.00  0.00           O
ATOM   5353  H   ASN A 509      18.172  59.974 -16.942  1.00  0.00           H
ATOM   5354  HA  ASN A 509      18.339  62.469 -18.455  1.00  0.00           H
ATOM   5355 1HB  ASN A 509      19.829  60.597 -18.954  1.00  0.00           H
ATOM   5356 2HB  ASN A 509      18.420  59.568 -19.308  1.00  0.00           H
ATOM   5357 1HD2 ASN A 509      18.706  60.444 -22.690  1.00  0.00           H
ATOM   5358 2HD2 ASN A 509      18.620  59.184 -21.480  1.00  0.00           H
ATOM   5359  N   VAL A 510      15.555  61.257 -17.873  1.00  0.00           N
ATOM   5360  CA  VAL A 510      14.177  61.671 -18.060  1.00  0.00           C
ATOM   5361  C   VAL A 510      14.204  63.194 -18.059  1.00  0.00           C
ATOM   5362  O   VAL A 510      14.877  63.801 -17.226  1.00  0.00           O
ATOM   5363  CB  VAL A 510      13.293  61.081 -16.953  1.00  0.00           C
ATOM   5364 CGI  VAL A 510      11.907  61.734 -16.850  1.00  0.00           C
ATOM   5365 CG2  VAL A 510      13.124  59.587 -17.245  1.00  0.00           C
ATOM   5366  H   VAL A 510      15.817  60.828 -16.997  1.00  0.00           H
ATOM   5367  HA  VAL A 510      13.791  61.244 -18.986  1.00  0.00           H
ATOM   5368  HB  VAL A 510      13.792  61.195 -15.991  1.00  0.00           H
ATOM   5369 1HG1 VAL A 510      11.342  61.263 -16.045  1.00  0.00           H
ATOM   5370 2HG1 VAL A 510      12.020  62.797 -16.639  1.00  0.00           H
ATOM   5371 3HG1 VAL A 510      11.373  61.605 -17.791  1.00  0.00           H
ATOM   5372 1HG2 VAL A 510      12.499  59.135 -16.475  1.00  0.00           H
ATOM   5373 2HG2 VAL A 510      12.651  59.458 -18.218  1.00  0.00           H
ATOM   5374 3HG2 VAL A 510      14.101  59.104 -17.249  1.00  0.00           H
ATOM   5375  N   LYS A 511      13.523  63.801 -19.022  1.00  0.00           N
ATOM   5376  CA  LYS A 511      13.549  65.225 -19.316  1.00  0.00           C
ATOM   5377  C   LYS A 511      12.113  65.667 -19.586  1.00  0.00           C
ATOM   5378  O   LYS A 511      11.861  66.612 -20.328  1.00  0.00           O
ATOM   5379  CB  LYS A 511      14.485  65.465 -20.506  1.00  0.00           C
ATOM   5380  CG  LYS A 511      15.933  65.190 -20.073  1.00  0.00           C
ATOM   5381  CD  LYS A 511      16.934  65.243 -21.226  1.00  0.00           C
ATOM   5382  CE  LYS A 511      16.615  64.190 -22.293  1.00  0.00           C
ATOM   5383  NZ  LYS A 511      17.819  63.776 -23.024  1.00  0.00          N1+
ATOM   5384  H   LYS A 511      12.920  63.265 -19.629  1.00  0.00           H
ATOM   5385  HA  LYS A 511      14.004  65.761 -18.483  1.00  0.00           H
ATOM   5386 1HB  LYS A 511      14.215  64.796 -21.322  1.00  0.00           H
ATOM   5387 2HB  LYS A 511      14.393  66.499 -20.839  1.00  0.00           H
ATOM   5388 1HG  LYS A 511      16.241  65.935 -19.340  1.00  0.00           H
ATOM   5389 2HG  LYS A 511      15.998  64.197 -19.630  1.00  0.00           H
ATOM   5390 1HD  LYS A 511      16.901  66.228 -21.692  1.00  0.00           H
ATOM   5391 2HD  LYS A 511      17.937  65.055 -20.845  1.00  0.00           H
ATOM   5392 1HE  LYS A 511      16.183  63.309 -21.817  1.00  0.00           H
ATOM   5393 2HE  LYS A 511      15.903  64.601 -23.009  1.00  0.00           H
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ATOM   5394 1HZ  LYS A 511     17.572  63.084 -23.717  1.00  0.00           H
ATOM   5395 2HZ  LYS A 511     18.228  64.579 -23.482  1.00  0.00           H
ATOM   5396 3HZ  LYS A 511     18.487  63.382 -22.378  1.00  0.00           H
ATOM   5397  N   HIS A 512     11.168  64.954 -18.976  1.00  0.00           N
ATOM   5398  CA  HIS A 512      9.847  65.473 -18.714  1.00  0.00           C
ATOM   5399  C   HIS A 512      9.274  64.706 -17.523  1.00  0.00           C
ATOM   5400  O   HIS A 512      9.035  63.502 -17.613  1.00  0.00           O
ATOM   5401  CB  HIS A 512      8.941  65.376 -19.950  1.00  0.00           C
ATOM   5402  CG  HIS A 512      7.733  66.275 -19.858  1.00  0.00           C
ATOM   5403  CD2 HIS A 512      7.419  67.299 -18.994  1.00  0.00           C
ATOM   5404  ND1 HIS A 512      6.667  66.213 -20.753  1.00  0.00           N
ATOM   5405  CE1 HIS A 512      5.857  67.251 -20.489  1.00  0.00           C
ATOM   5406  NE2 HIS A 512      6.261  67.925 -19.415  1.00  0.00           N
ATOM   5407  H   HIS A 512     11.363  64.009 -18.677  1.00  0.00           H
ATOM   5408  HA  HIS A 512      9.905  66.548 -18.543  1.00  0.00           H
ATOM   5409 1HB  HIS A 512      9.505  65.664 -20.837  1.00  0.00           H
ATOM   5410 2HB  HIS A 512      8.588  64.351 -20.062  1.00  0.00           H
ATOM   5411 HD2  HIS A 512      8.051  67.500 -18.143  1.00  0.00           H
ATOM   5412 HD1  HIS A 512      6.624  65.470 -21.436  1.00  0.00           H
ATOM   5413 HE1  HIS A 512      5.004  67.445 -21.121  1.00  0.00           H
ATOM   5414  N   VAL A 513      9.065  65.394 -16.407  1.00  0.00           N
ATOM   5415  CA  VAL A 513      8.251  64.911 -15.309  1.00  0.00           C
ATOM   5416  C   VAL A 513      6.906  65.608 -15.452  1.00  0.00           C
ATOM   5417  O   VAL A 513      6.859  66.809 -15.712  1.00  0.00           O
ATOM   5418  CB  VAL A 513      8.923  65.201 -13.955  1.00  0.00           C
ATOM   5419  CGI VAL A 513      7.926  65.132 -12.789  1.00  0.00           C
ATOM   5420  CG2 VAL A 513     10.025  64.163 -13.723  1.00  0.00           C
ATOM   5421  H   VAL A 513      9.485  66.306 -16.290  1.00  0.00           H
ATOM   5422  HA  VAL A 513      8.178  63.824 -15.361  1.00  0.00           H
ATOM   5423  HB  VAL A 513      9.360  66.200 -13.973  1.00  0.00           H
ATOM   5424 1HG1 VAL A 513      8.445  65.344 -11.854  1.00  0.00           H
ATOM   5425 2HG1 VAL A 513      7.137  65.868 -12.940  1.00  0.00           H
ATOM   5426 3HG1 VAL A 513      7.489  64.135 -12.743  1.00  0.00           H
ATOM   5427 1HG2 VAL A 513     10.511  64.357 -12.766  1.00  0.00           H
ATOM   5428 2HG2 VAL A 513      9.588  63.165 -13.712  1.00  0.00           H
ATOM   5429 3HG2 VAL A 513     10.762  64.229 -14.524  1.00  0.00           H
ATOM   5430  N   ILE A 514      5.826  64.854 -15.289  1.00  0.00           N
ATOM   5431  CA  ILE A 514      4.475  65.366 -15.337  1.00  0.00           C
ATOM   5432  C   ILE A 514      3.866  65.009 -13.983  1.00  0.00           C
ATOM   5433  O   ILE A 514      3.528  63.853 -13.733  1.00  0.00           O
ATOM   5434  CB  ILE A 514      3.728  64.733 -16.522  1.00  0.00           C
ATOM   5435  CGI ILE A 514      4.446  65.040 -17.852  1.00  0.00           C
ATOM   5436  CG2 ILE A 514      2.290  65.270 -16.560  1.00  0.00           C
ATOM   5437  CD1 ILE A 514      4.097  64.016 -18.932  1.00  0.00           C
ATOM   5438  H   ILE A 514      5.923  63.863 -15.119  1.00  0.00           H
ATOM   5439  HA  ILE A 514      4.500  66.439 -15.527  1.00  0.00           H
ATOM   5440  HB  ILE A 514      3.661  63.655 -16.375  1.00  0.00           H
ATOM   5441 1HG1 ILE A 514      4.148  66.027 -18.207  1.00  0.00           H
ATOM   5442 2HG1 ILE A 514      5.524  65.021 -17.697  1.00  0.00           H
ATOM   5443 1HG2 ILE A 514      1.757  64.823 -17.400  1.00  0.00           H
ATOM   5444 2HG2 ILE A 514      1.782  65.016 -15.631  1.00  0.00           H
ATOM   5445 3HG2 ILE A 514      2.310  66.353 -16.679  1.00  0.00           H
ATOM   5446 1HD1 ILE A 514      4.621  64.266 -19.854  1.00  0.00           H
ATOM   5447 2HD1 ILE A 514      4.399  63.022 -18.601  1.00  0.00           H
ATOM   5448 3HD1 ILE A 514      3.022  64.028 -19.111  1.00  0.00           H
ATOM   5449  N   ASN A 515      3.760  65.977 -13.078  1.00  0.00           N
ATOM   5450  CA  ASN A 515      3.193  65.709 -11.767  1.00  0.00           C
ATOM   5451  C   ASN A 515      1.682  65.684 -11.938  1.00  0.00           C
ATOM   5452  O   ASN A 515      1.066  66.724 -12.165  1.00  0.00           O
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ATOM   5453  CB  ASN A 515      3.607  66.762 -10.733  1.00  0.00           C
ATOM   5454  CG  ASN A 515      5.102  66.749 -10.450  1.00  0.00           C
ATOM   5455  ND2 ASN A 515      5.750  67.908 -10.451  1.00  0.00           N
ATOM   5456  OD1 ASN A 515      5.692  65.697 -10.225  1.00  0.00           O
ATOM   5457  H   ASN A 515      4.074  66.911 -13.299  1.00  0.00           H
ATOM   5458  HA  ASN A 515      3.578  64.760 -11.391  1.00  0.00           H
ATOM   5459  1HB ASN A 515      3.345  67.755 -11.101  1.00  0.00           H
ATOM   5460  2HB ASN A 515      3.087  66.574  -9.794  1.00  0.00           H
ATOM   5461  1HD2 ASN A 515      6.742  67.933 -10.266  1.00  0.00           H
ATOM   5462  2HD2 ASN A 515      5.250  68.766 -10.636  1.00  0.00           H
ATOM   5463  N   PHE A 516      1.093  64.497 -11.835  1.00  0.00           N
ATOM   5464  CA  PHE A 516     -0.340  64.301 -11.766  1.00  0.00           C
ATOM   5465  C   PHE A 516     -0.784  64.653 -10.350  1.00  0.00           C
ATOM   5466  O   PHE A 516     -1.845  65.250 -10.169  1.00  0.00           O
ATOM   5467  CB  PHE A 516     -0.642  62.839 -12.106  1.00  0.00           C
ATOM   5468  CG  PHE A 516     -2.103  62.445 -12.225  1.00  0.00           C
ATOM   5469  CD1 PHE A 516     -2.658  62.151 -13.487  1.00  0.00           C
ATOM   5470  CD2 PHE A 516     -2.919  62.325 -11.082  1.00  0.00           C
ATOM   5471  CE1 PHE A 516     -3.998  61.742 -13.605  1.00  0.00           C
ATOM   5472  CE2 PHE A 516     -4.261  61.928 -11.199  1.00  0.00           C
ATOM   5473  CZ  PHE A 516     -4.804  61.637 -12.461  1.00  0.00           C
ATOM   5474  H   PHE A 516      1.653  63.657 -11.801  1.00  0.00           H
ATOM   5475  HA  PHE A 516     -0.831  64.937 -12.502  1.00  0.00           H
ATOM   5476  1HB PHE A 516     -0.194  62.589 -13.068  1.00  0.00           H
ATOM   5477  2HB PHE A 516     -0.228  62.192 -11.333  1.00  0.00           H
ATOM   5478  HD1 PHE A 516     -2.053  62.239 -14.378  1.00  0.00           H
ATOM   5479  HD2 PHE A 516     -2.514  62.540 -10.104  1.00  0.00           H
ATOM   5480  HE1 PHE A 516     -4.408  61.508 -14.577  1.00  0.00           H
ATOM   5481  HE2 PHE A 516     -4.879  61.845 -10.318  1.00  0.00           H
ATOM   5482  HZ  PHE A 516     -5.837  61.334 -12.553  1.00  0.00           H
ATOM   5483  N   ASP A 517      0.049  64.288  -9.373  1.00  0.00           N
ATOM   5484  CA  ASP A 517     -0.114  64.659  -7.978  1.00  0.00           C
ATOM   5485  C   ASP A 517      1.172  65.377  -7.568  1.00  0.00           C
ATOM   5486  O   ASP A 517      2.277  64.825  -7.655  1.00  0.00           O
ATOM   5487  CB  ASP A 517     -0.334  63.437  -7.074  1.00  0.00           C
ATOM   5488  CG  ASP A 517     -1.627  62.689  -7.349  1.00  0.00           C
ATOM   5489  OD1 ASP A 517     -2.702  63.325  -7.287  1.00  0.00           O
ATOM   5490  OD2 ASP A 517     -1.539  61.462  -7.589  1.00  0.00          O1-
ATOM   5491  H   ASP A 517      0.855  63.716  -9.584  1.00  0.00           H
ATOM   5492  HA  ASP A 517     -0.976  65.319  -7.876  1.00  0.00           H
ATOM   5493  1HB ASP A 517      0.483  62.729  -7.215  1.00  0.00           H
ATOM   5494  2HB ASP A 517     -0.362  63.756  -6.032  1.00  0.00           H
ATOM   5495  N   LEU A 518      1.035  66.612  -7.100  1.00  0.00           N
ATOM   5496  CA  LEU A 518      2.109  67.337  -6.447  1.00  0.00           C
ATOM   5497  C   LEU A 518      2.206  66.800  -5.013  1.00  0.00           C
ATOM   5498  O   LEU A 518      1.298  66.109  -4.549  1.00  0.00           O
ATOM   5499  CB  LEU A 518      1.809  68.841  -6.546  1.00  0.00           C
ATOM   5500  CG  LEU A 518      2.370  69.457  -7.835  1.00  0.00           C
ATOM   5501  CD1 LEU A 518      1.668  70.796  -8.069  1.00  0.00           C
ATOM   5502  CD2 LEU A 518      3.887  69.683  -7.765  1.00  0.00           C
ATOM   5503  H   LEU A 518      0.151  67.091  -7.191  1.00  0.00           H
ATOM   5504  HA  LEU A 518      3.026  67.228  -7.025  1.00  0.00           H
ATOM   5505  1HB LEU A 518      0.731  68.998  -6.535  1.00  0.00           H
ATOM   5506  2HB LEU A 518      2.259  69.358  -5.699  1.00  0.00           H
ATOM   5507  HG  LEU A 518      2.195  68.777  -8.669  1.00  0.00           H
ATOM   5508  1HD1 LEU A 518      2.051  71.253  -8.982  1.00  0.00           H
ATOM   5509  2HD1 LEU A 518      0.595  70.631  -8.169  1.00  0.00           H
ATOM   5510  3HD1 LEU A 518      1.857  71.458  -7.225  1.00  0.00           H
ATOM   5511  1HD2 LEU A 518      4.234  70.120  -8.701  1.00  0.00           H
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ATOM   5512 2HD2 LEU A 518      4.116  70.359  -6.941  1.00  0.00           H
ATOM   5513 3HD2 LEU A 518      4.389  68.729  -7.601  1.00  0.00           H
ATOM   5514  N   PRO A 519      3.322  66.996  -4.306  1.00  0.00           N
ATOM   5515  CA  PRO A 519      3.506  66.379  -3.004  1.00  0.00           C
ATOM   5516  C   PRO A 519      2.497  66.882  -1.968  1.00  0.00           C
ATOM   5517  O   PRO A 519      2.177  68.067  -1.917  1.00  0.00           O
ATOM   5518  CB  PRO A 519      4.930  66.742  -2.591  1.00  0.00           C
ATOM   5519  CG  PRO A 519      5.199  68.048  -3.325  1.00  0.00           C
ATOM   5520  CD  PRO A 519      4.429  67.880  -4.628  1.00  0.00           C
ATOM   5521  HA  PRO A 519      3.394  65.299  -3.093  1.00  0.00           H
ATOM   5522 1HB  PRO A 519      4.976  66.861  -1.508  1.00  0.00           H
ATOM   5523 2HB  PRO A 519      5.612  65.949  -2.898  1.00  0.00           H
ATOM   5524 1HG  PRO A 519      4.832  68.883  -2.728  1.00  0.00           H
ATOM   5525 2HG  PRO A 519      6.271  68.160  -3.486  1.00  0.00           H
ATOM   5526 1HD  PRO A 519      5.046  67.425  -5.402  1.00  0.00           H
ATOM   5527 2HD  PRO A 519      4.040  68.833  -4.988  1.00  0.00           H
ATOM   5528  N   SER A 520      2.066  65.974  -1.094  1.00  0.00           N
ATOM   5529  CA  SER A 520      1.724  66.332   0.273  1.00  0.00           C
ATOM   5530  C   SER A 520      2.975  66.140   1.141  1.00  0.00           C
ATOM   5531  O   SER A 520      3.065  66.665   2.246  1.00  0.00           O
ATOM   5532  CB  SER A 520      0.581  65.428   0.743  1.00  0.00           C
ATOM   5533  OG  SER A 520     -0.398  65.330  -0.277  1.00  0.00           O
ATOM   5534  H   SER A 520      1.970  65.009  -1.374  1.00  0.00           H
ATOM   5535  HA  SER A 520      1.387  67.368   0.305  1.00  0.00           H
ATOM   5536 1HB  SER A 520      0.972  64.435   0.967  1.00  0.00           H
ATOM   5537 2HB  SER A 520      0.129  65.850   1.640  1.00  0.00           H
ATOM   5538  HG  SER A 520     -1.114  64.763   0.019  1.00  0.00           H
ATOM   5539  N   ASP A 521      3.948  65.382   0.628  1.00  0.00           N
ATOM   5540  CA  ASP A 521      5.257  65.167   1.209  1.00  0.00           C
ATOM   5541  C   ASP A 521      6.165  66.306   0.739  1.00  0.00           C
ATOM   5542  O   ASP A 521      7.161  66.082   0.058  1.00  0.00           O
ATOM   5543  CB  ASP A 521      5.768  63.764   0.823  1.00  0.00           C
ATOM   5544  CG  ASP A 521      5.802  63.422  -0.665  1.00  0.00           C
ATOM   5545  OD1 ASP A 521      4.922  63.893  -1.423  1.00  0.00           O
ATOM   5546  OD2 ASP A 521      6.636  62.549  -1.013  1.00  0.00           O1-
ATOM   5547  H   ASP A 521      3.801  64.895  -0.244  1.00  0.00           H
ATOM   5548  HA  ASP A 521      5.167  65.095   2.293  1.00  0.00           H
ATOM   5549 1HB  ASP A 521      6.793  63.641   1.175  1.00  0.00           H
ATOM   5550 2HB  ASP A 521      5.133  63.007   1.283  1.00  0.00           H
ATOM   5551  N   ILE A 522      5.752  67.528   1.097  1.00  0.00           N
ATOM   5552  CA  ILE A 522      6.267  68.838   0.705  1.00  0.00           C
ATOM   5553  C   ILE A 522      7.597  68.818  -0.064  1.00  0.00           C
ATOM   5554  O   ILE A 522      7.610  69.046  -1.277  1.00  0.00           O
ATOM   5555  CB  ILE A 522      6.208  69.823   1.898  1.00  0.00           C
ATOM   5556 CG1  ILE A 522      6.862  71.189   1.614  1.00  0.00           C
ATOM   5557 CG2  ILE A 522      6.776  69.262   3.213  1.00  0.00           C
ATOM   5558 CD1  ILE A 522      6.230  71.926   0.430  1.00  0.00           C
ATOM   5559  H   ILE A 522      4.971  67.632   1.729  1.00  0.00           H
ATOM   5560  HA  ILE A 522      5.466  69.426   0.258  1.00  0.00           H
ATOM   5561  HB  ILE A 522      5.175  69.928   2.232  1.00  0.00           H
ATOM   5562 1HG1 ILE A 522      6.763  71.829   2.490  1.00  0.00           H
ATOM   5563 2HG1 ILE A 522      7.918  71.046   1.386  1.00  0.00           H
ATOM   5564 1HG2 ILE A 522      6.695  70.016   3.996  1.00  0.00           H
ATOM   5565 2HG2 ILE A 522      6.212  68.376   3.504  1.00  0.00           H
ATOM   5566 3HG2 ILE A 522      7.823  68.996   3.073  1.00  0.00           H
ATOM   5567 1HD1 ILE A 522      6.737  72.880   0.283  1.00  0.00           H
ATOM   5568 2HD1 ILE A 522      6.330  71.320  -0.471  1.00  0.00           H
ATOM   5569 3HD1 ILE A 522      5.174  72.104   0.633  1.00  0.00           H
ATOM   5570  N   GLU A 523      8.719  68.593   0.625  1.00  0.00           N
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ATOM 5571 CA GLU A 523 10.041 68.763 0.051 1.00 0.00 C
ATOM 5572 C GLU A 523 10.263 67.861 -1.169 1.00 0.00 C
ATOM 5573 O GLU A 523 11.162 68.129 -1.967 1.00 0.00 O
ATOM 5574 CB GLU A 523 11.116 68.513 1.112 1.00 0.00 C
ATOM 5575 CG GLU A 523 11.144 69.566 2.228 1.00 0.00 C
ATOM 5576 CD GLU A 523 12.319 69.300 3.153 1.00 0.00 C
ATOM 5577 OE1 GLU A 523 12.074 68.849 4.289 1.00 0.00 O
ATOM 5578 OE2 GLU A 523 13.470 69.430 2.682 1.00 0.00 Ol-
ATOM 5579 H GLU A 523 8.668 68.291 1.587 1.00 0.00 H
ATOM 5580 HA GLU A 523 10.197 69.812 -0.201 1.00 0.00 H
ATOM 5581 1HB GLU A 523 10.943 67.547 1.585 1.00 0.00 H
ATOM 5582 2HB GLU A 523 12.100 68.516 0.642 1.00 0.00 H
ATOM 5583 IHG GLU A 523 11.248 70.558 1.789 1.00 0.00 H
ATOM 5584 2HG GLU A 523 10.217 69.516 2.798 1.00 0.00 H
ATOM 5585 N GLU A 524 9.454 66.810 -1.359 1.00 0.00 N
ATOM 5586 CA GLU A 524 9.599 65.970 -2.530 1.00 0.00 C
ATOM 5587 C GLU A 524 9.387 66.774 -3.817 1.00 0.00 C
ATOM 5588 O GLU A 524 9.786 66.321 -4.890 1.00 0.00 O
ATOM 5589 CB GLU A 524 8.717 64.706 -2.494 1.00 0.00 C
ATOM 5590 CG GLU A 524 9.551 63.542 -3.047 1.00 0.00 C
ATOM 5591 CD GLU A 524 8.787 62.331 -3.517 1.00 0.00 C
ATOM 5592 OE1 GLU A 524 9.193 61.228 -3.099 1.00 0.00 O
ATOM 5593 OE2 GLU A 524 7.954 62.482 -4.430 1.00 0.00 Ol-
ATOM 5594 H GLU A 524 8.735 66.597 -0.682 1.00 0.00 H
ATOM 5595 HA GLU A 524 10.552 65.443 -2.485 1.00 0.00 H
ATOM 5596 1HB GLU A 524 8.415 64.502 -1.467 1.00 0.00 H
ATOM 5597 2HB GLU A 524 7.831 64.863 -3.109 1.00 0.00 H
ATOM 5598 IHG GLU A 524 10.127 63.884 -3.907 1.00 0.00 H
ATOM 5599 2HG GLU A 524 10.231 63.183 -2.275 1.00 0.00 H
ATOM 5600 N TYR A 525 8.784 67.964 -3.735 1.00 0.00 N
ATOM 5601 CA TYR A 525 8.741 68.901 -4.846 1.00 0.00 C
ATOM 5602 C TYR A 525 10.147 69.057 -5.426 1.00 0.00 C
ATOM 5603 O TYR A 525 10.339 68.960 -6.638 1.00 0.00 O
ATOM 5604 CB TYR A 525 8.188 70.263 -4.392 1.00 0.00 C
ATOM 5605 CG TYR A 525 8.024 71.332 -5.465 1.00 0.00 C
ATOM 5606 CD1 TYR A 525 7.647 71.013 -6.787 1.00 0.00 C
ATOM 5607 CD2 TYR A 525 8.213 72.688 -5.135 1.00 0.00 C
ATOM 5608 CE1 TYR A 525 7.440 72.025 -7.740 1.00 0.00 C
ATOM 5609 CE2 TYR A 525 7.999 73.701 -6.086 1.00 0.00 C
ATOM 5610 CZ TYR A 525 7.590 73.379 -7.392 1.00 0.00 C
ATOM 5611 OH TYR A 525 7.307 74.359 -8.301 1.00 0.00 O
ATOM 5612 H TYR A 525 8.333 68.243 -2.876 1.00 0.00 H
ATOM 5613 HA TYR A 525 8.040 68.541 -5.599 1.00 0.00 H
ATOM 5614 1HB TYR A 525 7.197 70.127 -3.958 1.00 0.00 H
ATOM 5615 2HB TYR A 525 8.855 70.695 -3.646 1.00 0.00 H
ATOM 5616 HD1 TYR A 525 7.514 69.981 -7.076 1.00 0.00 H
ATOM 5617 HD2 TYR A 525 8.526 72.963 -4.139 1.00 0.00 H
ATOM 5618 HE1 TYR A 525 7.163 71.766 -8.751 1.00 0.00 H
ATOM 5619 HE2 TYR A 525 8.148 74.736 -5.815 1.00 0.00 H
ATOM 5620 HH TYR A 525 7.462 75.219 -7.904 1.00 0.00 H
ATOM 5621 N VAL A 526 11.132 69.246 -4.547 1.00 0.00 N
ATOM 5622 CA VAL A 526 12.514 69.488 -4.916 1.00 0.00 C
ATOM 5623 C VAL A 526 13.075 68.255 -5.641 1.00 0.00 C
ATOM 5624 O VAL A 526 14.034 68.357 -6.406 1.00 0.00 O
ATOM 5625 CB VAL A 526 13.336 69.878 -3.669 1.00 0.00 C
ATOM 5626 CGI VAL A 526 14.749 70.340 -4.055 1.00 0.00 C
ATOM 5627 CG2 VAL A 526 12.670 71.024 -2.890 1.00 0.00 C
ATOM 5628 H VAL A 526 10.937 69.224 -3.557 1.00 0.00 H
ATOM 5629 HA VAL A 526 12.579 70.401 -5.506 1.00 0.00 H

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ATOM   5630  HB  VAL A 526      13.420  69.019  -3.005  1.00  0.00           H
ATOM   5631 1HG1 VAL A 526      15.302  70.608  -3.155  1.00  0.00           H
ATOM   5632 2HG1 VAL A 526      15.267  69.533  -4.572  1.00  0.00           H
ATOM   5633 3HG1 VAL A 526      14.681  71.208  -4.711  1.00  0.00           H
ATOM   5634 1HG2 VAL A 526      13.277  71.272  -2.019  1.00  0.00           H
ATOM   5635 2HG2 VAL A 526      12.584  71.900  -3.533  1.00  0.00           H
ATOM   5636 3HG2 VAL A 526      11.678  70.714  -2.564  1.00  0.00           H
ATOM   5637  N   HIS A 527      12.487  67.077  -5.416  1.00  0.00           N
ATOM   5638  CA  HIS A 527      12.940  65.855  -6.049  1.00  0.00           C
ATOM   5639  C   HIS A 527      12.162  65.632  -7.342  1.00  0.00           C
ATOM   5640  O   HIS A 527      12.693  65.041  -8.277  1.00  0.00           O
ATOM   5641  CB  HIS A 527      12.767  64.610  -5.180  1.00  0.00           C
ATOM   5642  CG  HIS A 527      12.974  64.734  -3.701  1.00  0.00           C
ATOM   5643  CD2 HIS A 527      13.458  65.730  -2.891  1.00  0.00           C
ATOM   5644  ND1 HIS A 527      12.631  63.693  -2.847  1.00  0.00           N
ATOM   5645  CE1 HIS A 527      12.776  64.127  -1.589  1.00  0.00           C
ATOM   5646  NE2 HIS A 527      13.310  65.342  -1.576  1.00  0.00           N
ATOM   5647  H   HIS A 527      11.699  67.018  -4.787  1.00  0.00           H
ATOM   5648  HA  HIS A 527      14.006  65.930  -6.264  1.00  0.00           H
ATOM   5649 1HB  HIS A 527      11.752  64.229  -5.287  1.00  0.00           H
ATOM   5650 2HB  HIS A 527      13.477  63.845  -5.496  1.00  0.00           H
ATOM   5651  HD2 HIS A 527      13.867  66.630  -3.327  1.00  0.00           H
ATOM   5652  HD1 HIS A 527      12.336  62.804  -3.227  1.00  0.00           H
ATOM   5653  HE1 HIS A 527      12.472  63.502  -0.763  1.00  0.00           H
ATOM   5654  N   ARG A 528      10.894  66.035  -7.405  1.00  0.00           N
ATOM   5655  CA  ARG A 528      10.089  65.890  -8.610  1.00  0.00           C
ATOM   5656  C   ARG A 528      10.631  66.818  -9.702  1.00  0.00           C
ATOM   5657  O   ARG A 528      10.547  66.491 -10.882  1.00  0.00           O
ATOM   5658  CB  ARG A 528       8.593  66.087  -8.310  1.00  0.00           C
ATOM   5659  CG  ARG A 528       8.089  64.910  -7.458  1.00  0.00           C
ATOM   5660  CD  ARG A 528       6.596  64.940  -7.092  1.00  0.00           C
ATOM   5661  NE  ARG A 528       6.356  64.007  -5.979  1.00  0.00           N
ATOM   5662  CZ  ARG A 528       5.292  63.932  -5.174  1.00  0.00           C
ATOM   5663  NH1 ARG A 528       4.085  64.337  -5.578  1.00  0.00           N1+
ATOM   5664  NH2 ARG A 528       5.507  63.441  -3.960  1.00  0.00           N
ATOM   5665  H   ARG A 528      10.459  66.459  -6.598  1.00  0.00           H
ATOM   5666  HA  ARG A 528      10.035  64.837  -8.887  1.00  0.00           H
ATOM   5667 1HB  ARG A 528       8.451  67.020  -7.766  1.00  0.00           H
ATOM   5668 2HB  ARG A 528       8.037  66.125  -9.247  1.00  0.00           H
ATOM   5669 1HG  ARG A 528       8.252  63.976  -7.996  1.00  0.00           H
ATOM   5670 2HG  ARG A 528       8.633  64.885  -6.514  1.00  0.00           H
ATOM   5671 1HD  ARG A 528       6.315  65.949  -6.792  1.00  0.00           H
ATOM   5672 2HD  ARG A 528       6.004  64.640  -7.957  1.00  0.00           H
ATOM   5673  HE  ARG A 528       7.128  63.366  -5.857  1.00  0.00           H
ATOM   5674 1HH1 ARG A 528       3.295  64.271  -4.953  1.00  0.00           H
ATOM   5675 2HH1 ARG A 528       3.962  64.709  -6.509  1.00  0.00           H
ATOM   5676 1HH2 ARG A 528       4.742  63.359  -3.306  1.00  0.00           H
ATOM   5677 2HH2 ARG A 528       6.435  63.148  -3.691  1.00  0.00           H
ATOM   5678  N   ILE A 529      11.272  67.921  -9.309  1.00  0.00           N
ATOM   5679  CA  ILE A 529      12.034  68.783 -10.212  1.00  0.00           C
ATOM   5680  C   ILE A 529      13.512  68.349 -10.208  1.00  0.00           C
ATOM   5681  O   ILE A 529      14.406  69.061 -10.671  1.00  0.00           O
ATOM   5682  CB  ILE A 529      11.833  70.263  -9.827  1.00  0.00           C
ATOM   5683  CGI ILE A 529      12.606  70.629  -8.547  1.00  0.00           C
ATOM   5684  CG2 ILE A 529      10.332  70.566  -9.691  1.00  0.00           C
ATOM   5685  CD1 ILE A 529      12.333  72.045  -8.037  1.00  0.00           C
ATOM   5686  H   ILE A 529      11.246  68.202  -8.339  1.00  0.00           H
ATOM   5687  HA  ILE A 529      11.578  68.767 -11.202  1.00  0.00           H
ATOM   5688  HB  ILE A 529      12.112  70.899 -10.666  1.00  0.00           H
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ATOM   5689 1HG1 ILE A 529     12.331 69.941  -7.747  1.00  0.00        H
ATOM   5690 2HG1 ILE A 529     13.677  70.556  -8.736  1.00  0.00        H
ATOM   5691 1HG2 ILE A 529     10.195  71.613  -9.419  1.00  0.00        H
ATOM   5692 2HG2 ILE A 529      9.834  70.371 -10.641  1.00  0.00        H
ATOM   5693 3HG2 ILE A 529      9.900  69.931  -8.917  1.00  0.00        H
ATOM   5694 1HD1 ILE A 529     12.915  72.225  -7.133  1.00  0.00        H
ATOM   5695 2HD1 ILE A 529     12.618  72.768  -8.801  1.00  0.00        H
ATOM   5696 3HD1 ILE A 529     11.272  72.153  -7.812  1.00  0.00        H
ATOM   5697  N   GLY A 530     13.782  67.168  -9.654  1.00  0.00        N
ATOM   5698  CA  GLY A 530     15.089  66.725  -9.216  1.00  0.00        C
ATOM   5699  C   GLY A 530     15.520  65.525 -10.047  1.00  0.00        C
ATOM   5700  O   GLY A 530     16.499  65.605 -10.790  1.00  0.00        O
ATOM   5701  H   GLY A 530     13.041  66.496  -9.511  1.00  0.00        H
ATOM   5702 1HA  GLY A 530     15.808  67.534  -9.343  1.00  0.00        H
ATOM   5703 2HA  GLY A 530     15.043  66.443  -8.164  1.00  0.00        H
ATOM   5704  N   ARG A 531     14.771  64.417  -9.965  1.00  0.00        N
ATOM   5705  CA  ARG A 531     15.144  63.179 -10.635  1.00  0.00        C
ATOM   5706  C   ARG A 531     15.383  63.427 -12.138  1.00  0.00        C
ATOM   5707  O   ARG A 531     16.163  62.718 -12.772  1.00  0.00        O
ATOM   5708  CB  ARG A 531     14.124  62.032 -10.440  1.00  0.00        C
ATOM   5709  CG  ARG A 531     13.018  62.110  -9.371  1.00  0.00        C
ATOM   5710  CD  ARG A 531     13.469  62.000  -7.904  1.00  0.00        C
ATOM   5711  NE  ARG A 531     12.297  61.936  -7.006  1.00  0.00        N
ATOM   5712  CZ  ARG A 531     12.260  61.427  -5.758  1.00  0.00        C
ATOM   5713  NH1 ARG A 531     13.400  61.062  -5.160  1.00  0.00        N1+
ATOM   5714  NH2 ARG A 531     11.066  61.359  -5.158  1.00  0.00        N
ATOM   5715  H   ARG A 531     13.918  64.423  -9.424  1.00  0.00        H
ATOM   5716  HA  ARG A 531     16.012  62.744 -10.140  1.00  0.00        H
ATOM   5717 1HB  ARG A 531     13.565  61.881 -11.364  1.00  0.00        H
ATOM   5718 2HB  ARG A 531     14.653  61.114 -10.182  1.00  0.00        H
ATOM   5719 1HG  ARG A 531     12.501  63.066  -9.451  1.00  0.00        H
ATOM   5720 2HG  ARG A 531     12.306  61.299  -9.524  1.00  0.00        H
ATOM   5721 1HD  ARG A 531     14.064  61.096  -7.774  1.00  0.00        H
ATOM   5722 2HD  ARG A 531     14.069  62.871  -7.642  1.00  0.00        H
ATOM   5723  HE  ARG A 531     11.462  62.327  -7.417  1.00  0.00        H
ATOM   5724 1HH1 ARG A 531     13.380  60.681  -4.225  1.00  0.00        H
ATOM   5725 2HH1 ARG A 531     14.281  61.168  -5.643  1.00  0.00        H
ATOM   5726 1HH2 ARG A 531     10.991  60.985  -4.223  1.00  0.00        H
ATOM   5727 2HH2 ARG A 531     10.239  61.682  -5.640  1.00  0.00        H
ATOM   5728  N   THR A 532     14.718  64.435 -12.703  1.00  0.00        N
ATOM   5729  CA  THR A 532     14.865  64.839 -14.088  1.00  0.00        C
ATOM   5730  C   THR A 532     15.942  65.926 -14.198  1.00  0.00        C
ATOM   5731  O   THR A 532     15.924  66.902 -13.444  1.00  0.00        O
ATOM   5732  CB  THR A 532     13.499  65.311 -14.628  1.00  0.00        C
ATOM   5733  CG2 THR A 532     12.808  66.402 -13.797  1.00  0.00        C
ATOM   5734  OG1 THR A 532     13.615  65.791 -15.948  1.00  0.00        O
ATOM   5735  H   THR A 532     14.060  64.973 -12.158  1.00  0.00        H
ATOM   5736  HA  THR A 532     15.098  63.967 -14.699  1.00  0.00        H
ATOM   5737  HB  THR A 532     12.825  64.459 -14.709  1.00  0.00        H
ATOM   5738 1HG2 THR A 532     11.856  66.664 -14.260  1.00  0.00        H
ATOM   5739 2HG2 THR A 532     12.630  66.032 -12.787  1.00  0.00        H
ATOM   5740 3HG2 THR A 532     13.445  67.285 -13.753  1.00  0.00        H
ATOM   5741  HG1 THR A 532     12.755  66.079 -16.262  1.00  0.00        H
ATOM   5742  N   GLY A 533     16.869  65.784 -15.151  1.00  0.00        N
ATOM   5743  CA  GLY A 533     17.707  66.888 -15.601  1.00  0.00        C
ATOM   5744  C   GLY A 533     19.166  66.485 -15.793  1.00  0.00        C
ATOM   5745  O   GLY A 533     20.043  67.346 -15.847  1.00  0.00        O
ATOM   5746  H   GLY A 533     17.009  64.884 -15.588  1.00  0.00        H
ATOM   5747 1HA  GLY A 533     17.337  67.260 -16.556  1.00  0.00        H
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ATOM 5748 2HA GLY A 533 17.679 67.690 -14.864 1.00 0.00 H
ATOM 5749 N ARG A 534 19.450 65.188 -15.894 1.00 0.00 N
ATOM 5750 CA ARG A 534 20.799 64.674 -16.071 1.00 0.00 C
ATOM 5751 C ARG A 534 20.769 63.645 -17.202 1.00 0.00 C
ATOM 5752 O ARG A 534 20.855 62.449 -16.961 1.00 0.00 O
ATOM 5753 CB ARG A 534 21.274 64.064 -14.742 1.00 0.00 C
ATOM 5754 CG ARG A 534 21.518 65.121 -13.648 1.00 0.00 C
ATOM 5755 CD ARG A 534 21.439 64.498 -12.250 1.00 0.00 C
ATOM 5756 NE ARG A 534 20.069 64.025 -11.975 1.00 0.00 N
ATOM 5757 CZ ARG A 534 19.744 62.903 -11.320 1.00 0.00 C
ATOM 5758 NH1 ARG A 534 18.498 62.455 -11.380 1.00 0.00 N1+
ATOM 5759 NH2 ARG A 534 20.657 62.232 -10.631 1.00 0.00 N
ATOM 5760 H ARG A 534 18.708 64.505 -15.849 1.00 0.00 H
ATOM 5761 HA ARG A 534 21.476 65.499 -16.291 1.00 0.00 H
ATOM 5762 HXT ARG A 534 20.671 63.985 -18.222 1.00 0.00 H
ATOM 5763 1HB ARG A 534 20.520 63.370 -14.370 1.00 0.00 H
ATOM 5764 2HB ARG A 534 22.211 63.530 -14.901 1.00 0.00 H
ATOM 5765 1HG ARG A 534 22.508 65.559 -13.779 1.00 0.00 H
ATOM 5766 2HG ARG A 534 20.763 65.904 -13.724 1.00 0.00 H
ATOM 5767 1HD ARG A 534 22.125 63.653 -12.189 1.00 0.00 H
ATOM 5768 2HD ARG A 534 21.713 65.243 -11.503 1.00 0.00 H
ATOM 5769 HE ARG A 534 19.343 64.631 -12.330 1.00 0.00 H
ATOM 5770 1HH1 ARG A 534 18.241 61.610 -10.889 1.00 0.00 H
ATOM 5771 2HH1 ARG A 534 17.805 62.959 -11.915 1.00 0.00 H
ATOM 5772 1HH2 ARG A 534 20.400 61.387 -10.141 1.00 0.00 H
ATOM 5773 2HH2 ARG A 534 21.610 62.565 -10.596 1.00 0.00 H
ATOM 5774 N ASN A 537 19.113 68.471 -22.383 1.00 0.00 N
ATOM 5775 CA ASN A 537 19.295 67.883 -21.045 1.00 0.00 C
ATOM 5776 C ASN A 537 18.159 68.315 -20.113 1.00 0.00 C
ATOM 5777 O ASN A 537 17.958 67.724 -19.060 1.00 0.00 O
ATOM 5778 CB ASN A 537 20.649 68.285 -20.444 1.00 0.00 C
ATOM 5779 CG ASN A 537 20.894 67.602 -19.094 1.00 0.00 C
ATOM 5780 ND2 ASN A 537 21.268 68.362 -18.073 1.00 0.00 N
ATOM 5781 OD1 ASN A 537 20.753 66.389 -18.964 1.00 0.00 O
ATOM 5782 1H ASN A 537 19.868 68.178 -22.986 1.00 0.00 H
ATOM 5783 2H ASN A 537 18.233 68.161 -22.770 1.00 0.00 H
ATOM 5784 HA ASN A 537 19.337 66.797 -21.128 1.00 0.00 H
ATOM 5785 1HB ASN A 537 21.449 67.995 -21.125 1.00 0.00 H
ATOM 5786 2HB ASN A 537 20.674 69.364 -20.293 1.00 0.00 H
ATOM 5787 1HD2 ASN A 537 21.438 67.945 -17.169 1.00 0.00 H
ATOM 5788 2HD2 ASN A 537 21.383 69.357 -18.200 1.00 0.00 H
ATOM 5789 N LEU A 538 17.456 69.366 -20.534 1.00 0.00 N
ATOM 5790 CA LEU A 538 16.408 70.109 -19.836 1.00 0.00 C
ATOM 5791 C LEU A 538 15.661 69.278 -18.780 1.00 0.00 C
ATOM 5792 O LEU A 538 14.968 68.318 -19.115 1.00 0.00 O
ATOM 5793 CB LEU A 538 15.430 70.651 -20.890 1.00 0.00 C
ATOM 5794 CG LEU A 538 14.528 71.782 -20.370 1.00 0.00 C
ATOM 5795 CD1 LEU A 538 15.308 73.100 -20.271 1.00 0.00 C
ATOM 5796 CD2 LEU A 538 13.354 71.977 -21.336 1.00 0.00 C
ATOM 5797 H LEU A 538 17.624 69.749 -21.453 1.00 0.00 H
ATOM 5798 HA LEU A 538 16.839 70.994 -19.369 1.00 0.00 H
ATOM 5799 1HB LEU A 538 15.990 71.046 -21.738 1.00 0.00 H
ATOM 5800 2HB LEU A 538 14.778 69.846 -21.230 1.00 0.00 H
ATOM 5801 HG LEU A 538 14.155 71.524 -19.379 1.00 0.00 H
ATOM 5802 1HD1 LEU A 538 14.649 73.886 -19.901 1.00 0.00 H
ATOM 5803 2HD1 LEU A 538 16.146 72.977 -19.585 1.00 0.00 H
ATOM 5804 3HD1 LEU A 538 15.683 73.376 -21.257 1.00 0.00 H
ATOM 5805 1HD2 LEU A 538 12.711 72.778 -20.971 1.00 0.00 H
ATOM 5806 2HD2 LEU A 538 13.734 72.238 -22.324 1.00 0.00 H

ATOM 5807 3HD2 LEU A 538 12.779 71.053 -21.401 1.00 0.00 H
ATOM 5808 N GLY A 539 15.772 69.661 -17.509 1.00 0.00 N
ATOM 5809 CA GLY A 539 15.097 68.978 -16.420 1.00 0.00 C
ATOM 5810 C GLY A 539 13.700 69.564 -16.275 1.00 0.00 C
ATOM 5811 O GLY A 539 13.451 70.359 -15.372 1.00 0.00 O
ATOM 5812 H GLY A 539 16.345 70.458 -17.270 1.00 0.00 H
ATOM 5813 1HA GLY A 539 15.032 67.913 -16.642 1.00 0.00 H
ATOM 5814 2HA GLY A 539 15.658 69.122 -15.496 1.00 0.00 H
ATOM 5815 N LEU A 540 12.811 69.179 -17.189 1.00 0.00 N
ATOM 5816 CA LEU A 540 11.489 69.768 -17.306 1.00 0.00 C
ATOM 5817 C LEU A 540 10.535 69.049 -16.353 1.00 0.00 C
ATOM 5818 O LEU A 540 10.362 67.835 -16.456 1.00 0.00 O
ATOM 5819 CB LEU A 540 11.015 69.671 -18.767 1.00 0.00 C
ATOM 5820 CG LEU A 540 10.078 70.810 -19.210 1.00 0.00 C
ATOM 5821 CD1 LEU A 540 9.571 70.509 -20.625 1.00 0.00 C
ATOM 5822 CD2 LEU A 540 8.872 71.017 -18.287 1.00 0.00 C
ATOM 5823 H LEU A 540 13.044 68.445 -17.843 1.00 0.00 H
ATOM 5824 HA LEU A 540 11.546 70.835 -17.090 1.00 0.00 H
ATOM 5825 1HB LEU A 540 11.878 69.693 -19.432 1.00 0.00 H
ATOM 5826 2HB LEU A 540 10.470 68.738 -18.912 1.00 0.00 H
ATOM 5827 HG LEU A 540 10.618 71.757 -19.180 1.00 0.00 H
ATOM 5828 1HD1 LEU A 540 8.906 71.309 -20.951 1.00 0.00 H
ATOM 5829 2HD1 LEU A 540 10.418 70.440 -21.308 1.00 0.00 H
ATOM 5830 3HD1 LEU A 540 9.029 69.564 -20.624 1.00 0.00 H
ATOM 5831 1HD2 LEU A 540 8.261 71.836 -18.665 1.00 0.00 H
ATOM 5832 2HD2 LEU A 540 8.277 70.104 -18.256 1.00 0.00 H
ATOM 5833 3HD2 LEU A 540 9.220 71.258 -17.282 1.00 0.00 H
ATOM 5834 N ALA A 541 9.886 69.793 -15.464 1.00 0.00 N
ATOM 5835 CA ALA A 541 8.820 69.309 -14.612 1.00 0.00 C
ATOM 5836 C ALA A 541 7.579 70.160 -14.871 1.00 0.00 C
ATOM 5837 O ALA A 541 7.505 71.310 -14.440 1.00 0.00 O
ATOM 5838 CB ALA A 541 9.260 69.402 -13.152 1.00 0.00 C
ATOM 5839 H ALA A 541 10.126 70.768 -15.349 1.00 0.00 H
ATOM 5840 HA ALA A 541 8.628 68.259 -14.831 1.00 0.00 H
ATOM 5841 1HB ALA A 541 8.460 69.039 -12.507 1.00 0.00 H
ATOM 5842 2HB ALA A 541 10.152 68.795 -13.002 1.00 0.00 H
ATOM 5843 3HB ALA A 541 9.482 70.441 -12.905 1.00 0.00 H
ATOM 5844 N THR A 542 6.591 69.584 -15.543 1.00 0.00 N
ATOM 5845 CA THR A 542 5.274 70.175 -15.663 1.00 0.00 C
ATOM 5846 C THR A 542 4.426 69.562 -14.548 1.00 0.00 C
ATOM 5847 O THR A 542 4.615 68.399 -14.194 1.00 0.00 O
ATOM 5848 CB THR A 542 4.704 69.876 -17.060 1.00 0.00 C
ATOM 5849 CG2 THR A 542 3.350 70.555 -17.290 1.00 0.00 C
ATOM 5850 OG1 THR A 542 5.594 70.348 -18.055 1.00 0.00 O
ATOM 5851 H THR A 542 6.741 68.695 -15.999 1.00 0.00 H
ATOM 5852 HA THR A 542 5.352 71.258 -15.574 1.00 0.00 H
ATOM 5853 HB THR A 542 4.561 68.801 -17.173 1.00 0.00 H
ATOM 5854 1HG2 THR A 542 2.987 70.315 -18.290 1.00 0.00 H
ATOM 5855 2HG2 THR A 542 2.633 70.199 -16.550 1.00 0.00 H
ATOM 5856 3HG2 THR A 542 3.463 71.635 -17.195 1.00 0.00 H
ATOM 5857 HG1 THR A 542 5.232 70.159 -18.924 1.00 0.00 H
ATOM 5858 N SER A 543 3.491 70.319 -13.986 1.00 0.00 N
ATOM 5859 CA SER A 543 2.614 69.820 -12.949 1.00 0.00 C
ATOM 5860 C SER A 543 1.175 70.211 -13.251 1.00 0.00 C
ATOM 5861 O SER A 543 0.886 71.384 -13.493 1.00 0.00 O
ATOM 5862 CB SER A 543 3.064 70.397 -11.605 1.00 0.00 C
ATOM 5863 OG SER A 543 4.466 70.238 -11.445 1.00 0.00 O
ATOM 5864 H SER A 543 3.373 71.278 -14.281 1.00 0.00 H
ATOM 5865 HA SER A 543 2.708 68.736 -12.883 1.00 0.00 H

ATOM 5866 1HB SER A 543 2.819 71.458 -11.565 1.00 0.00 H
ATOM 5867 2HB SER A 543 2.553 69.875 -10.796 1.00 0.00 H
ATOM 5868 HG SER A 543 4.735 70.604 -10.599 1.00 0.00 H
ATOM 5869 N PHE A 544 0.284 69.229 -13.184 1.00 0.00 N
ATOM 5870 CA PHE A 544 -1.113 69.500 -12.939 1.00 0.00 C
ATOM 5871 C PHE A 544 -1.252 69.831 -11.449 1.00 0.00 C
ATOM 5872 O PHE A 544 -0.302 69.671 -10.677 1.00 0.00 O
ATOM 5873 CB PHE A 544 -1.953 68.277 -13.331 1.00 0.00 C
ATOM 5874 CG PHE A 544 -1.812 67.809 -14.772 1.00 0.00 C
ATOM 5875 CD1 PHE A 544 -1.796 68.735 -15.832 1.00 0.00 C
ATOM 5876 CD2 PHE A 544 -1.727 66.436 -15.081 1.00 0.00 C
ATOM 5877 CE1 PHE A 544 -1.712 68.303 -17.164 1.00 0.00 C
ATOM 5878 CE2 PHE A 544 -1.649 65.996 -16.413 1.00 0.00 C
ATOM 5879 CZ PHE A 544 -1.647 66.932 -17.459 1.00 0.00 C
ATOM 5880 H PHE A 544 0.579 68.270 -13.305 1.00 0.00 H
ATOM 5881 HA PHE A 544 -1.440 70.326 -13.571 1.00 0.00 H
ATOM 5882 1HB PHE A 544 -1.672 67.428 -12.708 1.00 0.00 H
ATOM 5883 2HB PHE A 544 -3.010 68.500 -13.186 1.00 0.00 H
ATOM 5884 HD1 PHE A 544 -1.847 69.794 -15.625 1.00 0.00 H
ATOM 5885 HD2 PHE A 544 -1.722 65.703 -14.287 1.00 0.00 H
ATOM 5886 HE1 PHE A 544 -1.697 69.025 -17.967 1.00 0.00 H
ATOM 5887 HE2 PHE A 544 -1.590 64.940 -16.631 1.00 0.00 H
ATOM 5888 HZ PHE A 544 -1.596 66.602 -18.486 1.00 0.00 H
ATOM 5889 N PHE A 545 -2.432 70.277 -11.038 1.00 0.00 N
ATOM 5890 CA PHE A 545 -2.714 70.737 -9.692 1.00 0.00 C
ATOM 5891 C PHE A 545 -4.229 70.679 -9.535 1.00 0.00 C
ATOM 5892 O PHE A 545 -4.950 70.862 -10.517 1.00 0.00 O
ATOM 5893 CB PHE A 545 -2.183 72.170 -9.517 1.00 0.00 C
ATOM 5894 CG PHE A 545 -2.466 72.826 -8.178 1.00 0.00 C
ATOM 5895 CD1 PHE A 545 -1.462 72.906 -7.193 1.00 0.00 C
ATOM 5896 CD2 PHE A 545 -3.730 73.387 -7.902 1.00 0.00 C
ATOM 5897 CE1 PHE A 545 -1.709 73.542 -5.964 1.00 0.00 C
ATOM 5898 CE2 PHE A 545 -3.984 74.007 -6.668 1.00 0.00 C
ATOM 5899 CZ PHE A 545 -2.971 74.094 -5.701 1.00 0.00 C
ATOM 5900 H PHE A 545 -3.210 70.311 -11.681 1.00 0.00 H
ATOM 5901 HA PHE A 545 -2.213 70.089 -8.973 1.00 0.00 H
ATOM 5902 1HB PHE A 545 -1.099 72.172 -9.631 1.00 0.00 H
ATOM 5903 2HB PHE A 545 -2.629 72.818 -10.271 1.00 0.00 H
ATOM 5904 HD1 PHE A 545 -0.489 72.474 -7.377 1.00 0.00 H
ATOM 5905 HD2 PHE A 545 -4.513 73.343 -8.644 1.00 0.00 H
ATOM 5906 HE1 PHE A 545 -0.927 73.607 -5.223 1.00 0.00 H
ATOM 5907 HE2 PHE A 545 -4.962 74.418 -6.461 1.00 0.00 H
ATOM 5908 HZ PHE A 545 -3.160 74.584 -4.757 1.00 0.00 H
ATOM 5909 N ASN A 546 -4.686 70.428 -8.313 1.00 0.00 N
ATOM 5910 CA ASN A 546 -6.076 70.428 -7.889 1.00 0.00 C
ATOM 5911 C ASN A 546 -6.100 70.285 -6.367 1.00 0.00 C
ATOM 5912 O ASN A 546 -5.037 70.124 -5.760 1.00 0.00 O
ATOM 5913 CB ASN A 546 -6.953 69.386 -8.607 1.00 0.00 C
ATOM 5914 CG ASN A 546 -6.495 67.932 -8.593 1.00 0.00 C
ATOM 5915 ND2 ASN A 546 -7.345 67.033 -9.073 1.00 0.00 N
ATOM 5916 ODl ASN A 546 -5.371 67.589 -8.225 1.00 0.00 O
ATOM 5917 H ASN A 546 -4.040 70.209 -7.568 1.00 0.00 H
ATOM 5918 HA ASN A 546 -6.578 71.310 -8.288 1.00 0.00 H
ATOM 5919 1HB ASN A 546 -7.945 69.374 -8.156 1.00 0.00 H
ATOM 5920 2HB ASN A 546 -7.037 69.646 -9.662 1.00 0.00 H
ATOM 5921 1HD2 ASN A 546 -7.091 66.055 -9.088 1.00 0.00 H
ATOM 5922 2HD2 ASN A 546 -8.245 67.326 -9.425 1.00 0.00 H
ATOM 5923 N GLU A 547 -7.293 70.409 -5.770 1.00 0.00 N
ATOM 5924 CA GLU A 547 -7.569 70.667 -4.357 1.00 0.00 C

ATOM 5925 C GLU A 547 -6.532 70.087 -3.385 1.00 0.00 C
ATOM 5926 O GLU A 547 -6.104 70.764 -2.453 1.00 0.00 O
ATOM 5927 CB GLU A 547 -8.983 70.179 -4.012 1.00 0.00 C
ATOM 5928 CG GLU A 547 -9.452 70.722 -2.656 1.00 0.00 C
ATOM 5929 CD GLU A 547 -10.840 70.216 -2.313 1.00 0.00 C
ATOM 5930 OE1 GLU A 547 -10.988 68.977 -2.261 1.00 0.00 O
ATOM 5931 OE2 GLU A 547 -11.721 71.079 -2.110 1.00 0.00 O1-
ATOM 5932 H GLU A 547 -8.140 70.322 -6.313 1.00 0.00 H
ATOM 5933 HA GLU A 547 -7.697 71.739 -4.201 1.00 0.00 H
ATOM 5934 1HB GLU A 547 -9.681 70.518 -4.778 1.00 0.00 H
ATOM 5935 2HB GLU A 547 -8.992 69.090 -3.969 1.00 0.00 H
ATOM 5936 1HG GLU A 547 -8.761 70.398 -1.876 1.00 0.00 H
ATOM 5937 2HG GLU A 547 -9.477 71.811 -2.688 1.00 0.00 H
ATOM 5938 N ARG A 548 -6.150 68.826 -3.599 1.00 0.00 N
ATOM 5939 CA ARG A 548 -5.126 68.112 -2.848 1.00 0.00 C
ATOM 5940 C ARG A 548 -3.976 69.020 -2.412 1.00 0.00 C
ATOM 5941 O ARG A 548 -3.484 68.921 -1.287 1.00 0.00 O
ATOM 5942 CB ARG A 548 -4.538 66.994 -3.721 1.00 0.00 C
ATOM 5943 CG ARG A 548 -5.576 65.919 -4.046 1.00 0.00 C
ATOM 5944 CD ARG A 548 -5.013 64.893 -5.034 1.00 0.00 C
ATOM 5945 NE ARG A 548 -6.068 63.930 -5.375 1.00 0.00 N
ATOM 5946 CZ ARG A 548 -6.280 63.424 -6.595 1.00 0.00 C
ATOM 5947 NH1 ARG A 548 -5.351 63.480 -7.542 1.00 0.00 N1+
ATOM 5948 NH2 ARG A 548 -7.455 62.853 -6.844 1.00 0.00 N
ATOM 5949 H ARG A 548 -6.582 68.285 -4.335 1.00 0.00 H
ATOM 5950 HA ARG A 548 -5.569 67.680 -1.950 1.00 0.00 H
ATOM 5951 1HB ARG A 548 -4.179 67.416 -4.660 1.00 0.00 H
ATOM 5952 2HB ARG A 548 -3.709 66.520 -3.196 1.00 0.00 H
ATOM 5953 1HG ARG A 548 -5.863 65.402 -3.131 1.00 0.00 H
ATOM 5954 2HG ARG A 548 -6.456 66.385 -4.490 1.00 0.00 H
ATOM 5955 1HD ARG A 548 -4.676 65.403 -5.937 1.00 0.00 H
ATOM 5956 2HD ARG A 548 -4.173 64.371 -4.577 1.00 0.00 H
ATOM 5957 HE ARG A 548 -6.657 63.652 -4.603 1.00 0.00 H
ATOM 5958 1HH1 ARG A 548 -5.537 63.090 -8.455 1.00 0.00 H
ATOM 5959 2HH1 ARG A 548 -4.459 63.912 -7.349 1.00 0.00 H
ATOM 5960 1HH2 ARG A 548 -7.644 62.462 -7.756 1.00 0.00 H
ATOM 5961 2HH2 ARG A 548 -8.159 62.810 -6.121 1.00 0.00 H
ATOM 5962 N ASN A 549 -3.494 69.846 -3.337 1.00 0.00 N
ATOM 5963 CA ASN A 549 -2.240 70.557 -3.176 1.00 0.00 C
ATOM 5964 C ASN A 549 -2.491 72.015 -2.819 1.00 0.00 C
ATOM 5965 O ASN A 549 -1.551 72.807 -2.783 1.00 0.00 O
ATOM 5966 CB ASN A 549 -1.382 70.394 -4.431 1.00 0.00 C
ATOM 5967 CG ASN A 549 -0.988 68.935 -4.626 1.00 0.00 C
ATOM 5968 ND2 ASN A 549 -0.090 68.405 -3.804 1.00 0.00 N
ATOM 5969 OD1 ASN A 549 -1.476 68.264 -5.531 1.00 0.00 O
ATOM 5970 H ASN A 549 -4.006 69.998 -4.194 1.00 0.00 H
ATOM 5971 HA ASN A 549 -1.619 70.038 -2.446 1.00 0.00 H
ATOM 5972 1HB ASN A 549 -1.945 70.726 -5.303 1.00 0.00 H
ATOM 5973 2HB ASN A 549 -0.477 70.993 -4.333 1.00 0.00 H
ATOM 5974 1HD2 ASN A 549 0.188 67.440 -3.913 1.00 0.00 H
ATOM 5975 2HD2 ASN A 549 0.316 68.967 -3.069 1.00 0.00 H
ATOM 5976 N ILE A 550 -3.733 72.367 -2.469 1.00 0.00 N
ATOM 5977 CA ILE A 550 -4.015 73.646 -1.828 1.00 0.00 C
ATOM 5978 C ILE A 550 -3.178 73.743 -0.545 1.00 0.00 C
ATOM 5979 O ILE A 550 -2.795 74.826 -0.105 1.00 0.00 O
ATOM 5980 CB ILE A 550 -5.525 73.816 -1.570 1.00 0.00 C
ATOM 5981 CGI ILE A 550 -6.289 74.008 -2.895 1.00 0.00 C
ATOM 5982 CG2 ILE A 550 -5.841 74.969 -0.606 1.00 0.00 C
ATOM 5983 CD1 ILE A 550 -6.171 75.416 -3.492 1.00 0.00 C

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ATOM   5984  H   ILE A 550     -4.505   71.741  -2.648  1.00  0.00           H
ATOM   5985  HA  ILE A 550      -3.828  74.456  -2.533  1.00  0.00           H
ATOM   5986  HB  ILE A 550      -5.896  72.961  -1.005  1.00  0.00           H
ATOM   5987  1HG1 ILE A 550     -5.904  73.312  -3.641  1.00  0.00           H
ATOM   5988  2HG1 ILE A 550     -7.350  73.817  -2.734  1.00  0.00           H
ATOM   5989  1HG2 ILE A 550     -6.919  75.039  -0.463  1.00  0.00           H
ATOM   5990  2HG2 ILE A 550     -5.359  74.782   0.354  1.00  0.00           H
ATOM   5991  3HG2 ILE A 550     -5.468  75.904  -1.023  1.00  0.00           H
ATOM   5992  1HD1 ILE A 550     -6.737  75.466  -4.422  1.00  0.00           H
ATOM   5993  2HD1 ILE A 550     -6.569  76.145  -2.786  1.00  0.00           H
ATOM   5994  3HD1 ILE A 550     -5.123  75.640  -3.693  1.00  0.00           H
ATOM   5995  N   ASN A 551      -2.861  72.584   0.032  1.00  0.00           N
ATOM   5996  CA  ASN A 551      -2.063  72.446   1.238  1.00  0.00           C
ATOM   5997  C   ASN A 551      -0.641  72.992   1.070  1.00  0.00           C
ATOM   5998  O   ASN A 551       0.089  73.044   2.054  1.00  0.00           O
ATOM   5999  CB  ASN A 551      -1.995  70.965   1.636  1.00  0.00           C
ATOM   6000  CG  ASN A 551      -3.335  70.449   2.144  1.00  0.00           C
ATOM   6001  ND2 ASN A 551      -4.042  69.652   1.351  1.00  0.00           N
ATOM   6002  OD1 ASN A 551      -3.753  70.775   3.250  1.00  0.00           O
ATOM   6003  H   ASN A 551      -3.182  71.715  -0.371  1.00  0.00           H
ATOM   6004  HA  ASN A 551      -2.553  72.968   2.060  1.00  0.00           H
ATOM   6005  1HB ASN A 551      -1.707  70.369   0.770  1.00  0.00           H
ATOM   6006  2HB ASN A 551      -1.257  70.834   2.427  1.00  0.00           H
ATOM   6007  1HD2 ASN A 551     -4.935  69.294   1.661  1.00  0.00           H
ATOM   6008  2HD2 ASN A 551     -3.688  69.404   0.438  1.00  0.00           H
ATOM   6009  N   ILE A 552      -0.209  73.338  -0.149  1.00  0.00           N
ATOM   6010  CA  ILE A 552       1.137  73.842  -0.406  1.00  0.00           C
ATOM   6011  C   ILE A 552       1.083  75.020  -1.387  1.00  0.00           C
ATOM   6012  O   ILE A 552       1.973  75.188  -2.224  1.00  0.00           O
ATOM   6013  CB  ILE A 552       2.054  72.705  -0.910  1.00  0.00           C
ATOM   6014  CG1 ILE A 552      1.516  72.051  -2.197  1.00  0.00           C
ATOM   6015  CG2 ILE A 552       2.260  71.643   0.181  1.00  0.00           C
ATOM   6016  CD1 ILE A 552       2.609  71.292  -2.952  1.00  0.00           C
ATOM   6017  H   ILE A 552      -0.824  73.257  -0.945  1.00  0.00           H
ATOM   6018  HA  ILE A 552       1.615  74.101   0.538  1.00  0.00           H
ATOM   6019  HB  ILE A 552       3.063  73.090  -1.058  1.00  0.00           H
ATOM   6020  1HG1 ILE A 552      0.724  71.346  -1.943  1.00  0.00           H
ATOM   6021  2HG1 ILE A 552      1.118  72.821  -2.857  1.00  0.00           H
ATOM   6022  1HG2 ILE A 552      2.910  70.853  -0.197  1.00  0.00           H
ATOM   6023  2HG2 ILE A 552      2.721  72.103   1.055  1.00  0.00           H
ATOM   6024  3HG2 ILE A 552      1.297  71.217   0.461  1.00  0.00           H
ATOM   6025  1HD1 ILE A 552      2.187  70.846  -3.852  1.00  0.00           H
ATOM   6026  2HD1 ILE A 552      3.407  71.982  -3.227  1.00  0.00           H
ATOM   6027  3HD1 ILE A 552      3.014  70.506  -2.313  1.00  0.00           H
ATOM   6028  N   THR A 553       0.048  75.858  -1.298  1.00  0.00           N
ATOM   6029  CA  THR A 553      -0.076  77.005  -2.191  1.00  0.00           C
ATOM   6030  C   THR A 553       0.860  78.137  -1.740  1.00  0.00           C
ATOM   6031  O   THR A 553       0.417  79.236  -1.414  1.00  0.00           O
ATOM   6032  CB  THR A 553      -1.543  77.464  -2.290  1.00  0.00           C
ATOM   6033  CG2 THR A 553      -1.815  78.210  -3.599  1.00  0.00           C
ATOM   6034  OG1 THR A 553      -2.400  76.349  -2.295  1.00  0.00           O
ATOM   6035  H   THR A 553      -0.668  75.705  -0.603  1.00  0.00           H
ATOM   6036  HA  THR A 553       0.104  76.687  -3.218  1.00  0.00           H
ATOM   6037  HB  THR A 553      -1.759  78.167  -1.486  1.00  0.00           H
ATOM   6038  1HG2 THR A 553     -2.860  78.518  -3.632  1.00  0.00           H
ATOM   6039  2HG2 THR A 553     -1.175  79.091  -3.655  1.00  0.00           H
ATOM   6040  3HG2 THR A 553     -1.603  77.553  -4.443  1.00  0.00           H
ATOM   6041  HG1 THR A 553      -3.311  76.645  -2.356  1.00  0.00           H
ATOM   6042  N   LYS A 554       2.170  77.897  -1.770  1.00  0.00           N
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ATOM   6043  CA  LYS A 554      3.163  78.918  -1.495  1.00  0.00      C
ATOM   6044  C   LYS A 554      4.530  78.439  -1.969  1.00  0.00      C
ATOM   6045  O   LYS A 554      5.025  78.933  -2.977  1.00  0.00      O
ATOM   6046  CB  LYS A 554      3.153  79.379  -0.022  1.00  0.00      C
ATOM   6047  CG  LYS A 554      2.858  80.885   0.083  1.00  0.00      C
ATOM   6048  CD  LYS A 554      4.001  81.717  -0.522  1.00  0.00      C
ATOM   6049  CE  LYS A 554      3.586  83.175  -0.766  1.00  0.00      C
ATOM   6050  NZ  LYS A 554      4.608  83.872  -1.567  1.00  0.00      N1+
ATOM   6051  H   LYS A 554      2.509  76.971  -1.990  1.00  0.00      H
ATOM   6052  HA  LYS A 554      2.833  79.868  -1.916  1.00  0.00      H
ATOM   6053 1HB  LYS A 554      2.384  78.833   0.525  1.00  0.00      H
ATOM   6054 2HB  LYS A 554      4.126  79.182   0.428  1.00  0.00      H
ATOM   6055 1HG  LYS A 554      1.938  81.113  -0.455  1.00  0.00      H
ATOM   6056 2HG  LYS A 554      2.743  81.161   1.131  1.00  0.00      H
ATOM   6057 1HD  LYS A 554      4.852  81.716   0.159  1.00  0.00      H
ATOM   6058 2HD  LYS A 554      4.300  81.285  -1.477  1.00  0.00      H
ATOM   6059 1HE  LYS A 554      2.638  83.198  -1.304  1.00  0.00      H
ATOM   6060 2HE  LYS A 554      3.475  83.686   0.190  1.00  0.00      H
ATOM   6061 1HZ  LYS A 554      4.322  84.829  -1.719  1.00  0.00      H
ATOM   6062 2HZ  LYS A 554      5.489  83.859  -1.074  1.00  0.00      H
ATOM   6063 3HZ  LYS A 554      4.714  83.407  -2.457  1.00  0.00      H
ATOM   6064  N   ASP A 555      5.127  77.464  -1.285  1.00  0.00      N
ATOM   6065  CA  ASP A 555      6.433  76.886  -1.592  1.00  0.00      C
ATOM   6066  C   ASP A 555      6.515  76.528  -3.075  1.00  0.00      C
ATOM   6067  O   ASP A 555      7.537  76.713  -3.738  1.00  0.00      O
ATOM   6068  CB  ASP A 555      6.629  75.606  -0.770  1.00  0.00      C
ATOM   6069  CG  ASP A 555      6.448  75.832   0.720  1.00  0.00      C
ATOM   6070  OD1 ASP A 555      7.447  75.676   1.450  1.00  0.00      O
ATOM   6071  OD2 ASP A 555      5.298  76.159   1.092  1.00  0.00      Ol-
ATOM   6072  H   ASP A 555      4.672  77.062  -0.477  1.00  0.00      H
ATOM   6073  HA  ASP A 555      7.214  77.613  -1.369  1.00  0.00      H
ATOM   6074 1HB  ASP A 555      5.902  74.857  -1.084  1.00  0.00      H
ATOM   6075 2HB  ASP A 555      7.637  75.223  -0.928  1.00  0.00      H
ATOM   6076  N   LEU A 556      5.400  75.986  -3.569  1.00  0.00      N
ATOM   6077  CA  LEU A 556      5.162  75.593  -4.944  1.00  0.00      C
ATOM   6078  C   LEU A 556      5.563  76.699  -5.931  1.00  0.00      C
ATOM   6079  O   LEU A 556      5.988  76.408  -7.052  1.00  0.00      O
ATOM   6080  CB  LEU A 556      3.674  75.231  -5.059  1.00  0.00      C
ATOM   6081  CG  LEU A 556      3.219  74.698  -6.425  1.00  0.00      C
ATOM   6082  CD1 LEU A 556      3.922  73.390  -6.796  1.00  0.00      C
ATOM   6083  CD2 LEU A 556      1.709  74.448  -6.354  1.00  0.00      C
ATOM   6084  H   LEU A 556      4.612  75.811  -2.962  1.00  0.00      H
ATOM   6085  HA  LEU A 556      5.703  74.671  -5.158  1.00  0.00      H
ATOM   6086 1HB  LEU A 556      3.432  74.454  -4.334  1.00  0.00      H
ATOM   6087 2HB  LEU A 556      3.068  76.115  -4.861  1.00  0.00      H
ATOM   6088  HG  LEU A 556      3.445  75.434  -7.197  1.00  0.00      H
ATOM   6089 1HD1 LEU A 556      3.569  73.050  -7.770  1.00  0.00      H
ATOM   6090 2HD1 LEU A 556      4.998  73.554  -6.838  1.00  0.00      H
ATOM   6091 3HD1 LEU A 556      3.699  72.631  -6.045  1.00  0.00      H
ATOM   6092 1HD2 LEU A 556      1.357  74.068  -7.313  1.00  0.00      H
ATOM   6093 2HD2 LEU A 556      1.497  73.716  -5.574  1.00  0.00      H
ATOM   6094 3HD2 LEU A 556      1.196  75.382  -6.124  1.00  0.00      H
ATOM   6095  N   LEU A 557      5.395  77.955  -5.517  1.00  0.00      N
ATOM   6096  CA  LEU A 557      5.710  79.156  -6.267  1.00  0.00      C
ATOM   6097  C   LEU A 557      7.040  79.716  -5.772  1.00  0.00      C
ATOM   6098  O   LEU A 557      7.927  80.004  -6.570  1.00  0.00      O
ATOM   6099  CB  LEU A 557      4.599  80.197  -6.054  1.00  0.00      C
ATOM   6100  CG  LEU A 557      4.803  81.486  -6.871  1.00  0.00      C
ATOM   6101  CD1 LEU A 557      4.322  81.314  -8.317  1.00  0.00      C
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ATOM   6102  CD2 LEU A 557      4.023  82.628  -6.215  1.00  0.00           C
ATOM   6103  H   LEU A 557      5.014  78.137  -4.599  1.00  0.00           H
ATOM   6104  HA  LEU A 557      5.787  78.913  -7.327  1.00  0.00           H
ATOM   6105  1HB  LEU A 557     3.640  79.772  -6.350  1.00  0.00           H
ATOM   6106  2HB  LEU A 557     4.562  80.480  -5.002  1.00  0.00           H
ATOM   6107  HG  LEU A 557      5.860  81.749  -6.877  1.00  0.00           H
ATOM   6108  1HD1 LEU A 557     4.481  82.243  -8.865  1.00  0.00           H
ATOM   6109  2HD1 LEU A 557     4.883  80.511  -8.794  1.00  0.00           H
ATOM   6110  3HD1 LEU A 557     3.261  81.067  -8.320  1.00  0.00           H
ATOM   6111  1HD2 LEU A 557     4.165  83.543  -6.791  1.00  0.00           H
ATOM   6112  2HD2 LEU A 557     2.963  82.377  -6.188  1.00  0.00           H
ATOM   6113  3HD2 LEU A 557     4.386  82.780  -5.198  1.00  0.00           H
ATOM   6114  N   ASP A 558      7.165  79.946  -4.467  1.00  0.00           N
ATOM   6115  CA  ASP A 558      8.219  80.799  -3.942  1.00  0.00           C
ATOM   6116  C   ASP A 558      9.590  80.164  -4.180  1.00  0.00           C
ATOM   6117  O   ASP A 558     10.591  80.870  -4.293  1.00  0.00           O
ATOM   6118  CB  ASP A 558      7.985  81.132  -2.461  1.00  0.00           C
ATOM   6119  CG  ASP A 558      6.951  82.228  -2.263  1.00  0.00           C
ATOM   6120  OD1 ASP A 558      6.040  82.376  -3.107  1.00  0.00           O
ATOM   6121  OD2 ASP A 558      7.007  82.938  -1.234  1.00  0.00           Ol-
ATOM   6122  H   ASP A 558      6.519  79.523  -3.816  1.00  0.00           H
ATOM   6123  HA  ASP A 558      8.128  81.797  -4.371  1.00  0.00           H
ATOM   6124  1HB  ASP A 558     7.633  80.243  -1.939  1.00  0.00           H
ATOM   6125  2HB  ASP A 558     8.919  81.470  -2.012  1.00  0.00           H
ATOM   6126  N   LEU A 559      9.654  78.835  -4.296  1.00  0.00           N
ATOM   6127  CA  LEU A 559     10.892  78.148  -4.630  1.00  0.00           C
ATOM   6128  C   LEU A 559     11.444  78.650  -5.972  1.00  0.00           C
ATOM   6129  O   LEU A 559     12.655  78.634  -6.201  1.00  0.00           O
ATOM   6130  CB  LEU A 559     10.644  76.632  -4.663  1.00  0.00           C
ATOM   6131  CG  LEU A 559     11.890  75.789  -4.989  1.00  0.00           C
ATOM   6132  CD1 LEU A 559     12.992  75.955  -3.934  1.00  0.00           C
ATOM   6133  CD2 LEU A 559     11.495  74.312  -5.075  1.00  0.00           C
ATOM   6134  H   LEU A 559      8.826  78.275  -4.150  1.00  0.00           H
ATOM   6135  HA  LEU A 559     11.617  78.293  -3.828  1.00  0.00           H
ATOM   6136  1HB  LEU A 559     10.283  76.301  -3.689  1.00  0.00           H
ATOM   6137  2HB  LEU A 559     9.897  76.403  -5.424  1.00  0.00           H
ATOM   6138  HG  LEU A 559     12.283  76.082  -5.963  1.00  0.00           H
ATOM   6139  1HD1 LEU A 559     13.851  75.343  -4.206  1.00  0.00           H
ATOM   6140  2HD1 LEU A 559     13.293  77.002  -3.885  1.00  0.00           H
ATOM   6141  3HD1 LEU A 559     12.614  75.640  -2.962  1.00  0.00           H
ATOM   6142  1HD2 LEU A 559     12.375  73.712  -5.306  1.00  0.00           H
ATOM   6143  2HD2 LEU A 559     11.078  73.991  -4.121  1.00  0.00           H
ATOM   6144  3HD2 LEU A 559     10.750  74.179  -5.860  1.00  0.00           H
ATOM   6145  N   LEU A 560     10.563  79.077  -6.878  1.00  0.00           N
ATOM   6146  CA  LEU A 560     10.945  79.551  -8.198  1.00  0.00           C
ATOM   6147  C   LEU A 560     11.771  80.833  -8.086  1.00  0.00           C
ATOM   6148  O   LEU A 560     12.526  81.165  -9.002  1.00  0.00           O
ATOM   6149  CB  LEU A 560      9.702  79.811  -9.062  1.00  0.00           C
ATOM   6150  CG  LEU A 560      8.733  78.620  -9.181  1.00  0.00           C
ATOM   6151  CD1 LEU A 560      7.471  79.093  -9.901  1.00  0.00           C
ATOM   6152  CD2 LEU A 560      9.329  77.448  -9.960  1.00  0.00           C
ATOM   6153  H   LEU A 560      9.577  79.081  -6.661  1.00  0.00           H
ATOM   6154  HA  LEU A 560     11.515  78.777  -8.712  1.00  0.00           H
ATOM   6155  1HB  LEU A 560     9.131  80.637  -8.638  1.00  0.00           H
ATOM   6156  2HB  LEU A 560     10.011  80.066 -10.076  1.00  0.00           H
ATOM   6157  HG  LEU A 560      8.485  78.252  -8.186  1.00  0.00           H
ATOM   6158  1HD1 LEU A 560     6.772  78.262  -9.995  1.00  0.00           H
ATOM   6159  2HD1 LEU A 560     7.005  79.896  -9.330  1.00  0.00           H
ATOM   6160  3HD1 LEU A 560     7.734  79.460 -10.894  1.00  0.00           H
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ATOM   6161 1HD2 LEU A 560      8.601  76.638 -10.011  1.00  0.00           H
ATOM   6162 2HD2 LEU A 560      9.583  77.773 -10.969  1.00  0.00           H
ATOM   6163 3HD2 LEU A 560     10.228  77.096  -9.455  1.00  0.00           H
ATOM   6164  N   VAL A 561     11.602  81.568  -6.984  1.00  0.00           N
ATOM   6165  CA  VAL A 561     12.263  82.842  -6.768  1.00  0.00           C
ATOM   6166  C   VAL A 561     13.740  82.594  -6.457  1.00  0.00           C
ATOM   6167  O   VAL A 561     14.571  83.465  -6.709  1.00  0.00           O
ATOM   6168  CB  VAL A 561     11.542  83.644  -5.666  1.00  0.00           C
ATOM   6169  CGI VAL A 561     12.158  85.038  -5.481  1.00  0.00           C
ATOM   6170  CG2 VAL A 561     10.054  83.819  -6.005  1.00  0.00           C
ATOM   6171  H   VAL A 561     10.990  81.242  -6.249  1.00  0.00           H
ATOM   6172  HA  VAL A 561     12.102  83.486  -7.632  1.00  0.00           H
ATOM   6173  HB  VAL A 561     11.606  83.104  -4.721  1.00  0.00           H
ATOM   6174 1HG1 VAL A 561     11.622  85.572  -4.696  1.00  0.00           H
ATOM   6175 2HG1 VAL A 561     13.206  84.939  -5.202  1.00  0.00           H
ATOM   6176 3HG1 VAL A 561     12.082  85.596  -6.415  1.00  0.00           H
ATOM   6177 1HG2 VAL A 561      9.565  84.388  -5.214  1.00  0.00           H
ATOM   6178 2HG2 VAL A 561      9.956  84.354  -6.950  1.00  0.00           H
ATOM   6179 3HG2 VAL A 561      9.583  82.840  -6.092  1.00  0.00           H
ATOM   6180  N   GLU A 562     14.076  81.402  -5.949  1.00  0.00           N
ATOM   6181  CA  GLU A 562     15.442  80.930  -6.033  1.00  0.00           C
ATOM   6182  C   GLU A 562     15.606  80.412  -7.457  1.00  0.00           C
ATOM   6183  O   GLU A 562     16.422  80.936  -8.207  1.00  0.00           O
ATOM   6184  CB  GLU A 562     15.763  79.851  -4.980  1.00  0.00           C
ATOM   6185  CG  GLU A 562     17.276  79.724  -4.697  1.00  0.00           C
ATOM   6186  CD  GLU A 562     18.116  79.457  -5.938  1.00  0.00           C
ATOM   6187  OE1 GLU A 562     17.856  78.457  -6.641  1.00  0.00           O
ATOM   6188  OE2 GLU A 562     18.984  80.292  -6.276  1.00  0.00           Ol-
ATOM   6189  H   GLU A 562     13.375  80.827  -5.504  1.00  0.00           H
ATOM   6190  HA  GLU A 562     16.124  81.742  -5.780  1.00  0.00           H
ATOM   6191 1HB  GLU A 562     15.267  80.099  -4.042  1.00  0.00           H
ATOM   6192 2HB  GLU A 562     15.408  78.882  -5.333  1.00  0.00           H
ATOM   6193 1HG  GLU A 562     17.642  80.650  -4.254  1.00  0.00           H
ATOM   6194 2HG  GLU A 562     17.449  78.898  -4.007  1.00  0.00           H
ATOM   6195  N   ALA A 563     14.864  79.364  -7.821  1.00  0.00           N
ATOM   6196  CA  ALA A 563     15.291  78.356  -8.784  1.00  0.00           C
ATOM   6197  C   ALA A 563     15.539  78.861 -10.213  1.00  0.00           C
ATOM   6198  O   ALA A 563     16.009  78.083 -11.040  1.00  0.00           O
ATOM   6199  CB  ALA A 563     14.315  77.177  -8.765  1.00  0.00           C
ATOM   6200  H   ALA A 563     13.945  79.233  -7.422  1.00  0.00           H
ATOM   6201  HA  ALA A 563     16.156  77.821  -8.391  1.00  0.00           H
ATOM   6202 1HB  ALA A 563     14.637  76.426  -9.486  1.00  0.00           H
ATOM   6203 2HB  ALA A 563     14.294  76.737  -7.768  1.00  0.00           H
ATOM   6204 3HB  ALA A 563     13.316  77.527  -9.028  1.00  0.00           H
ATOM   6205  N   LYS A 564     15.239  80.126 -10.521  1.00  0.00           N
ATOM   6206  CA  LYS A 564     15.471  80.764 -11.814  1.00  0.00           C
ATOM   6207  C   LYS A 564     14.652  80.046 -12.894  1.00  0.00           C
ATOM   6208  O   LYS A 564     15.190  79.216 -13.623  1.00  0.00           O
ATOM   6209  CB  LYS A 564     16.977  80.770 -12.167  1.00  0.00           C
ATOM   6210  CG  LYS A 564     17.860  81.539 -11.165  1.00  0.00           C
ATOM   6211  CD  LYS A 564     19.238  80.886 -10.921  1.00  0.00           C
ATOM   6212  CE  LYS A 564     19.205  79.558 -10.135  1.00  0.00           C
ATOM   6213  NZ  LYS A 564     18.668  79.717  -8.771  1.00  0.00           N1+
ATOM   6214  H   LYS A 564     14.815  80.727  -9.829  1.00  0.00           H
ATOM   6215  HA  LYS A 564     15.219  81.822 -11.748  1.00  0.00           H
ATOM   6216 1HB  LYS A 564     17.348  79.745 -12.197  1.00  0.00           H
ATOM   6217 2HB  LYS A 564     17.121  81.236 -13.142  1.00  0.00           H
ATOM   6218 1HG  LYS A 564     18.040  82.547 -11.538  1.00  0.00           H
ATOM   6219 2HG  LYS A 564     17.353  81.594 -10.201  1.00  0.00           H
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ATOM   6220 1HD  LYS A 564      19.712  80.669 -11.878  1.00  0.00           H
ATOM   6221 2HD  LYS A 564      19.868  81.569 -10.351  1.00  0.00           H
ATOM   6222 1HE  LYS A 564      18.574  78.841 -10.660  1.00  0.00           H
ATOM   6223 2HE  LYS A 564      20.216  79.160 -10.051  1.00  0.00           H
ATOM   6224 1HZ  LYS A 564      18.669  78.822  -8.303  1.00  0.00           H
ATOM   6225 2HZ  LYS A 564      19.245  80.366  -8.256  1.00  0.00           H
ATOM   6226 3HZ  LYS A 564      17.724  80.070  -8.820  1.00  0.00           H
ATOM   6227  N   GLN A 565      13.361  80.361 -13.005  1.00  0.00           N
ATOM   6228  CA  GLN A 565      12.396  79.505 -13.684  1.00  0.00           C
ATOM   6229  C   GLN A 565      11.388  80.320 -14.491  1.00  0.00           C
ATOM   6230  O   GLN A 565      11.268  81.532 -14.323  1.00  0.00           O
ATOM   6231  CB  GLN A 565      11.624  78.704 -12.627  1.00  0.00           C
ATOM   6232  CG  GLN A 565      12.522  77.753 -11.834  1.00  0.00           C
ATOM   6233  CD  GLN A 565      13.087  76.666 -12.733  1.00  0.00           C
ATOM   6234  NE2 GLN A 565      14.401  76.536 -12.836  1.00  0.00           N
ATOM   6235  OE1 GLN A 565      12.324  75.969 -13.390  1.00  0.00           O
ATOM   6236  H   GLN A 565      13.015  81.224 -12.609  1.00  0.00           H
ATOM   6237  HA  GLN A 565      12.919  78.848 -14.379  1.00  0.00           H
ATOM   6238 1HB  GLN A 565      11.159  79.390 -11.919  1.00  0.00           H
ATOM   6239 2HB  GLN A 565      10.853  78.107 -13.114  1.00  0.00           H
ATOM   6240 1HG  GLN A 565      13.350  78.312 -11.399  1.00  0.00           H
ATOM   6241 2HG  GLN A 565      11.943  77.284 -11.039  1.00  0.00           H
ATOM   6242 1HE2 GLN A 565      14.793  75.819 -13.429  1.00  0.00           H
ATOM   6243 2HE2 GLN A 565      15.011  77.155 -12.321  1.00  0.00           H
ATOM   6244  N   GLU A 566      10.633  79.610 -15.329  1.00  0.00           N
ATOM   6245  CA  GLU A 566       9.396  80.090 -15.910  1.00  0.00           C
ATOM   6246  C   GLU A 566       8.364  80.271 -14.786  1.00  0.00           C
ATOM   6247  O   GLU A 566       8.512  79.695 -13.707  1.00  0.00           O
ATOM   6248  CB  GLU A 566       8.920  79.056 -16.939  1.00  0.00           C
ATOM   6249  CG  GLU A 566       9.970  78.771 -18.028  1.00  0.00           C
ATOM   6250  CD  GLU A 566       9.524  77.609 -18.888  1.00  0.00           C
ATOM   6251  OE1 GLU A 566       9.498  76.470 -18.375  1.00  0.00           O
ATOM   6252  OE2 GLU A 566       9.095  77.827 -20.042  1.00  0.00           Ol-
ATOM   6253  H   GLU A 566      10.914  78.677 -15.594  1.00  0.00           H
ATOM   6254  HA  GLU A 566       9.577  81.037 -16.419  1.00  0.00           H
ATOM   6255 1HB  GLU A 566       8.699  78.116 -16.435  1.00  0.00           H
ATOM   6256 2HB  GLU A 566       8.020  79.423 -17.433  1.00  0.00           H
ATOM   6257 1HG  GLU A 566      10.093  79.653 -18.655  1.00  0.00           H
ATOM   6258 2HG  GLU A 566      10.922  78.523 -17.559  1.00  0.00           H
ATOM   6259  N   VAL A 567       7.311  81.048 -15.041  1.00  0.00           N
ATOM   6260  CA  VAL A 567       6.393  81.519 -14.014  1.00  0.00           C
ATOM   6261  C   VAL A 567       5.008  80.902 -14.258  1.00  0.00           C
ATOM   6262  O   VAL A 567       4.434  81.090 -15.329  1.00  0.00           O
ATOM   6263  CB  VAL A 567       6.327  83.057 -14.061  1.00  0.00           C
ATOM   6264  CGI VAL A 567       5.444  83.599 -12.930  1.00  0.00           C
ATOM   6265  CG2 VAL A 567       7.726  83.677 -13.924  1.00  0.00           C
ATOM   6266  H   VAL A 567       7.117  81.340 -15.989  1.00  0.00           H
ATOM   6267  HA  VAL A 567       6.773  81.240 -13.031  1.00  0.00           H
ATOM   6268  HB  VAL A 567       5.919  83.374 -15.021  1.00  0.00           H
ATOM   6269 1HG1 VAL A 567       5.412  84.688 -12.984  1.00  0.00           H
ATOM   6270 2HG1 VAL A 567       4.434  83.202 -13.035  1.00  0.00           H
ATOM   6271 3HG1 VAL A 567       5.856  83.295 -11.969  1.00  0.00           H
ATOM   6272 1HG2 VAL A 567       7.648  84.764 -13.960  1.00  0.00           H
ATOM   6273 2HG2 VAL A 567       8.165  83.377 -12.972  1.00  0.00           H
ATOM   6274 3HG2 VAL A 567       8.360  83.331 -14.740  1.00  0.00           H
ATOM   6275  N   PRO A 568       4.440  80.187 -13.277  1.00  0.00           N
ATOM   6276  CA  PRO A 568       3.067  79.711 -13.337  1.00  0.00           C
ATOM   6277  C   PRO A 568       2.072  80.863 -13.131  1.00  0.00           C
ATOM   6278  O   PRO A 568       1.406  80.939 -12.097  1.00  0.00           O
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ATOM   6279  CB  PRO A 568      2.965  78.650 -12.233  1.00  0.00           C
ATOM   6280  CG  PRO A 568      4.390  78.118 -12.122  1.00  0.00           C
ATOM   6281  CD  PRO A 568      5.205  79.392 -12.332  1.00  0.00           C
ATOM   6282  HA  PRO A 568      2.889  79.234 -14.301  1.00  0.00           H
ATOM   6283 1HB  PRO A 568      2.622  79.117 -11.310  1.00  0.00           H
ATOM   6284 2HB  PRO A 568      2.256  77.879 -12.534  1.00  0.00           H
ATOM   6285 1HG  PRO A 568      4.535  77.670 -11.139  1.00  0.00           H
ATOM   6286 2HG  PRO A 568      4.559  77.366 -12.892  1.00  0.00           H
ATOM   6287 1HD  PRO A 568      6.187  79.173 -12.751  1.00  0.00           H
ATOM   6288 2HD  PRO A 568      5.324  79.948 -11.401  1.00  0.00           H
ATOM   6289  N   SER A 569      1.983  81.771 -14.102  1.00  0.00           N
ATOM   6290  CA  SER A 569      1.220  82.996 -13.953  1.00  0.00           C
ATOM   6291  C   SER A 569     -0.274  82.724 -13.756  1.00  0.00           C
ATOM   6292  O   SER A 569     -1.025  82.592 -14.720  1.00  0.00           O
ATOM   6293  CB  SER A 569      1.492  83.920 -15.140  1.00  0.00           C
ATOM   6294  OG  SER A 569      2.876  84.216 -15.195  1.00  0.00           O
ATOM   6295  H   SER A 569      2.457  81.619 -14.980  1.00  0.00           H
ATOM   6296  HA  SER A 569      1.645  83.593 -13.146  1.00  0.00           H
ATOM   6297 1HB  SER A 569      1.188  83.426 -16.063  1.00  0.00           H
ATOM   6298 2HB  SER A 569      0.926  84.844 -15.019  1.00  0.00           H
ATOM   6299  HG  SER A 569      3.050  84.797 -15.940  1.00  0.00           H
ATOM   6300  N   TRP A 570     -0.678  82.674 -12.486  1.00  0.00           N
ATOM   6301  CA  TRP A 570     -1.984  82.399 -11.910  1.00  0.00           C
ATOM   6302  C   TRP A 570     -1.711  82.073 -10.437  1.00  0.00           C
ATOM   6303  O   TRP A 570     -2.362  82.579  -9.521  1.00  0.00           O
ATOM   6304  CB  TRP A 570     -2.727  81.241 -12.599  1.00  0.00           C
ATOM   6305  CG  TRP A 570     -2.107  79.879 -12.487  1.00  0.00           C
ATOM   6306  CD1 TRP A 570     -1.190  79.346 -13.325  1.00  0.00           C
ATOM   6307  CD2 TRP A 570     -2.343  78.865 -11.465  1.00  0.00           C
ATOM   6308  CE2 TRP A 570     -1.532  77.729 -11.757  1.00  0.00           C
ATOM   6309  CE3 TRP A 570     -3.153  78.786 -10.309  1.00  0.00           C
ATOM   6310  NE1 TRP A 570     -0.839  78.079 -12.898  1.00  0.00           N
ATOM   6311  CZ2 TRP A 570     -1.550  76.581 -10.951  1.00  0.00           C
ATOM   6312  CZ3 TRP A 570     -3.162  77.644  -9.488  1.00  0.00           C
ATOM   6313  CH2 TRP A 570     -2.364  76.537  -9.810  1.00  0.00           C
ATOM   6314  H   TRP A 570     -0.020  82.847 -11.740  1.00  0.00           H
ATOM   6315  HA  TRP A 570     -2.628  83.270 -12.035  1.00  0.00           H
ATOM   6316 1HB  TRP A 570     -3.726  81.145 -12.173  1.00  0.00           H
ATOM   6317 2HB  TRP A 570     -2.806  81.442 -13.667  1.00  0.00           H
ATOM   6318  HD1 TRP A 570     -0.846  79.912 -14.179  1.00  0.00           H
ATOM   6319  HE3 TRP A 570     -3.787  79.617 -10.036  1.00  0.00           H
ATOM   6320  HE1 TRP A 570     -0.154  77.545 -13.413  1.00  0.00           H
ATOM   6321  HZ2 TRP A 570     -0.936  75.730 -11.209  1.00  0.00           H
ATOM   6322  HZ3 TRP A 570     -3.785  77.618  -8.606  1.00  0.00           H
ATOM   6323  HH2 TRP A 570     -2.374  75.654  -9.187  1.00  0.00           H
ATOM   6324  N   LEU A 571     -0.684  81.257 -10.198  1.00  0.00           N
ATOM   6325  CA  LEU A 571     -0.310  80.826  -8.865  1.00  0.00           C
ATOM   6326  C   LEU A 571      0.301  82.010  -8.113  1.00  0.00           C
ATOM   6327  O   LEU A 571      0.222  82.081  -6.892  1.00  0.00           O
ATOM   6328  CB  LEU A 571      0.648  79.635  -8.972  1.00  0.00           C
ATOM   6329  CG  LEU A 571      1.046  79.027  -7.618  1.00  0.00           C
ATOM   6330  CD1 LEU A 571     -0.145  78.402  -6.882  1.00  0.00           C
ATOM   6331  CD2 LEU A 571      2.112  77.951 -7.848  1.00  0.00           C
ATOM   6332  H   LEU A 571     -0.126  80.911 -10.965  1.00  0.00           H
ATOM   6333  HA  LEU A 571     -1.183  80.416  -8.357  1.00  0.00           H
ATOM   6334 1HB  LEU A 571      0.179  78.842  -9.554  1.00  0.00           H
ATOM   6335 2HB  LEU A 571      1.568  79.951 -9.464  1.00  0.00           H
ATOM   6336  HG  LEU A 571      1.482  79.800  -6.985  1.00  0.00           H
ATOM   6337 1HD1 LEU A 571      0.191  77.987  -5.932  1.00  0.00           H
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ATOM 6338 2HD1 LEU A 571 -0.901 79.166 -6.698 1.00 0.00 H
ATOM 6339 3HD1 LEU A 571 -0.574 77.608 -7.493 1.00 0.00 H
ATOM 6340 1HD2 LEU A 571 2.400 77.514 -6.892 1.00 0.00 H
ATOM 6341 2HD2 LEU A 571 1.709 77.173 -8.496 1.00 0.00 H
ATOM 6342 3HD2 LEU A 571 2.986 78.400 -8.320 1.00 0.00 H
ATOM 6343 N GLU A 572 0.852 82.980 -8.844 1.00 0.00 N
ATOM 6344 CA GLU A 572 1.341 84.233 -8.285 1.00 0.00 C
ATOM 6345 C GLU A 572 0.182 85.156 -7.876 1.00 0.00 C
ATOM 6346 O GLU A 572 0.393 86.314 -7.523 1.00 0.00 O
ATOM 6347 CB GLU A 572 2.340 84.906 -9.241 1.00 0.00 C
ATOM 6348 CG GLU A 572 2.060 84.678 -10.734 1.00 0.00 C
ATOM 6349 CD GLU A 572 2.971 85.526 -11.614 1.00 0.00 C
ATOM 6350 OE1 GLU A 572 3.935 86.094 -11.064 1.00 0.00 O
ATOM 6351 OE2 GLU A 572 2.695 85.568 -12.832 1.00 0.00 Ol-
ATOM 6352 H GLU A 572 0.949 82.867 -9.843 1.00 0.00 H
ATOM 6353 HA GLU A 572 2.044 84.023 -7.479 1.00 0.00 H
ATOM 6354 1HB GLU A 572 2.328 85.984 -9.082 1.00 0.00 H
ATOM 6355 2HB GLU A 572 3.342 84.522 -9.049 1.00 0.00 H
ATOM 6356 1HG GLU A 572 2.226 83.629 -10.980 1.00 0.00 H
ATOM 6357 2HG GLU A 572 1.026 84.944 -10.955 1.00 0.00 H
ATOM 6358 N ASN A 573 -1.058 84.665 -7.907 1.00 0.00 N
ATOM 6359 CA ASN A 573 -2.196 85.306 -7.268 1.00 0.00 C
ATOM 6360 C ASN A 573 -2.767 84.332 -6.245 1.00 0.00 C
ATOM 6361 O ASN A 573 -3.040 84.729 -5.117 1.00 0.00 O
ATOM 6362 CB ASN A 573 -3.264 85.719 -8.290 1.00 0.00 C
ATOM 6363 CG ASN A 573 -2.961 87.009 -9.052 1.00 0.00 C
ATOM 6364 ND2 ASN A 573 -1.744 87.543 -8.999 1.00 0.00 N
ATOM 6365 OD1 ASN A 573 -3.840 87.549 -9.716 1.00 0.00 O
ATOM 6366 H ASN A 573 -1.247 83.801 -8.394 1.00 0.00 H
ATOM 6367 HA ASN A 573 -1.877 86.242 -6.810 1.00 0.00 H
ATOM 6368 1HB ASN A 573 -3.376 84.933 -9.037 1.00 0.00 H
ATOM 6369 2HB ASN A 573 -4.215 85.873 -7.780 1.00 0.00 H
ATOM 6370 1HD2 ASN A 573 -1.545 88.396 -9.503 1.00 0.00 H
ATOM 6371 2HD2 ASN A 573 -1.020 87.096 -8.455 1.00 0.00 H
ATOM 6372 N MET A 574 -2.938 83.056 -6.604 1.00 0.00 N
ATOM 6373 CA MET A 574 -3.536 82.100 -5.674 1.00 0.00 C
ATOM 6374 C MET A 574 -2.607 81.775 -4.499 1.00 0.00 C
ATOM 6375 O MET A 574 -3.063 81.293 -3.469 1.00 0.00 O
ATOM 6376 CB MET A 574 -4.021 80.838 -6.395 1.00 0.00 C
ATOM 6377 CG MET A 574 -5.100 81.186 -7.429 1.00 0.00 C
ATOM 6378 SD MET A 574 -6.083 79.784 -8.027 1.00 0.00 S
ATOM 6379 CE MET A 574 -7.156 79.513 -6.589 1.00 0.00 C
ATOM 6380 H MET A 574 -2.653 82.747 -7.523 1.00 0.00 H
ATOM 6381 HA MET A 574 -4.518 82.459 -5.365 1.00 0.00 H
ATOM 6382 1HB MET A 574 -3.182 80.367 -6.907 1.00 0.00 H
ATOM 6383 2HB MET A 574 -4.441 80.142 -5.669 1.00 0.00 H
ATOM 6384 1HG MET A 574 -5.805 81.895 -6.995 1.00 0.00 H
ATOM 6385 2HG MET A 574 -4.633 81.632 -8.307 1.00 0.00 H
ATOM 6386 1HE MET A 574 -7.829 78.680 -6.789 1.00 0.00 H
ATOM 6387 2HE MET A 574 -6.544 79.284 -5.716 1.00 0.00 H
ATOM 6388 3HE MET A 574 -7.740 80.413 -6.396 1.00 0.00 H
ATOM 6389 N ALA A 575 -1.315 82.091 -4.595 1.00 0.00 N
ATOM 6390 CA ALA A 575 -0.416 82.022 -3.447 1.00 0.00 C
ATOM 6391 C ALA A 575 -0.664 83.189 -2.483 1.00 0.00 C
ATOM 6392 O ALA A 575 0.094 83.389 -1.534 1.00 0.00 O
ATOM 6393 CB ALA A 575 1.038 81.992 -3.924 1.00 0.00 C
ATOM 6394 H ALA A 575 -0.932 82.389 -5.481 1.00 0.00 H
ATOM 6395 HA ALA A 575 -0.534 81.059 -2.950 1.00 0.00 H
ATOM 6396 1HB ALA A 575 1.703 81.940 -3.062 1.00 0.00 H

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ATOM   6397 2HB  ALA A 575       1.196   81.119  -4.557  1.00  0.00          H
ATOM   6398 3HB  ALA A 575       1.252   82.896  -4.493  1.00  0.00          H
ATOM   6399  N   TYR A 576      -1.701   83.985  -2.747  1.00  0.00          N
ATOM   6400  CA  TYR A 576      -2.199   85.064  -1.919  1.00  0.00          C
ATOM   6401  C   TYR A 576      -3.732   85.020  -1.989  1.00  0.00          C
ATOM   6402  O   TYR A 576      -4.396   86.058  -1.981  1.00  0.00          O
ATOM   6403  CB  TYR A 576      -1.628   86.397  -2.427  1.00  0.00          C
ATOM   6404  CG  TYR A 576      -0.124   86.376  -2.638  1.00  0.00          C
ATOM   6405  CD1 TYR A 576       0.757   86.560  -1.557  1.00  0.00          C
ATOM   6406  CD2 TYR A 576       0.416   86.131  -3.915  1.00  0.00          C
ATOM   6407  CE1 TYR A 576       2.147   86.477  -1.745  1.00  0.00          C
ATOM   6408  CE2 TYR A 576       1.806   86.048  -4.105  1.00  0.00          C
ATOM   6409  CZ  TYR A 576       2.686   86.210  -3.018  1.00  0.00          C
ATOM   6410  OH  TYR A 576       4.037   86.113  -3.190  1.00  0.00          O
ATOM   6411  H   TYR A 576      -2.226   83.863  -3.601  1.00  0.00          H
ATOM   6412  HA  TYR A 576      -1.829   84.941  -0.900  1.00  0.00          H
ATOM   6413 1HB  TYR A 576      -2.086   86.649  -3.383  1.00  0.00          H
ATOM   6414 2HB  TYR A 576      -1.842   87.184  -1.704  1.00  0.00          H
ATOM   6415  HDl  TYR A 576       0.367   86.768  -0.572  1.00  0.00          H
ATOM   6416  HD2 TYR A 576      -0.240   86.004  -4.764  1.00  0.00          H
ATOM   6417  HE1 TYR A 576       2.815   86.618  -0.907  1.00  0.00          H
ATOM   6418  HE2 TYR A 576       2.205   85.858  -5.090  1.00  0.00          H
ATOM   6419  HH  TYR A 576       4.230   85.929  -4.112  1.00  0.00          H
ATOM   6420  N   GLU A 577      -4.277   83.803  -2.085  1.00  0.00          N
ATOM   6421  CA  GLU A 577      -5.700   83.521  -2.197  1.00  0.00          C
ATOM   6422  C   GLU A 577      -6.494   84.232  -1.089  1.00  0.00          C
ATOM   6423  O   GLU A 577      -6.017   84.390   0.036  1.00  0.00          O
ATOM   6424  CB  GLU A 577      -5.886   81.993  -2.171  1.00  0.00          C
ATOM   6425  CG  GLU A 577      -7.323   81.463  -2.094  1.00  0.00          C
ATOM   6426  CD  GLU A 577      -8.184   81.877  -3.272  1.00  0.00          C
ATOM   6427  OE1 GLU A 577      -8.841   80.984  -3.840  1.00  0.00          O
ATOM   6428  OE2 GLU A 577      -8.304   83.098  -3.488  1.00  0.00          Ol-
ATOM   6429  H   GLU A 577      -3.686   82.984  -2.085  1.00  0.00          H
ATOM   6430  HA  GLU A 577      -6.051   83.802  -3.190  1.00  0.00          H
ATOM   6431 1HB  GLU A 577      -5.465   81.560  -3.078  1.00  0.00          H
ATOM   6432 2HB  GLU A 577      -5.377   81.579  -1.300  1.00  0.00          H
ATOM   6433 IHG  GLU A 577      -7.308   80.374  -2.067  1.00  0.00          H
ATOM   6434 2HG  GLU A 577      -7.802   81.842  -1.191  1.00  0.00          H
ATOM   6435  N   HIS A 578      -7.710   84.665  -1.417  1.00  0.00          N
ATOM   6436  CA  HIS A 578      -8.659   85.329  -0.539  1.00  0.00          C
ATOM   6437  C   HIS A 578     -10.078   84.816  -0.843  1.00  0.00          C
ATOM   6438  O   HIS A 578     -11.063   85.502  -0.560  1.00  0.00          O
ATOM   6439  CB  HIS A 578      -8.569   86.853  -0.742  1.00  0.00          C
ATOM   6440  CG  HIS A 578      -7.452   87.542   0.004  1.00  0.00          C
ATOM   6441  CD2 HIS A 578      -7.475   88.455   1.030  1.00  0.00          C
ATOM   6442  ND1 HIS A 578      -6.106   87.352  -0.276  1.00  0.00          N
ATOM   6443  CE1 HIS A 578      -5.390   88.110   0.568  1.00  0.00          C
ATOM   6444  NE2 HIS A 578      -6.182   88.820   1.372  1.00  0.00          N
ATOM   6445  H   HIS A 578      -8.053   84.543  -2.359  1.00  0.00          H
ATOM   6446  HA  HIS A 578      -8.390   85.138   0.499  1.00  0.00          H
ATOM   6447 1HB  HIS A 578      -8.414   87.072  -1.798  1.00  0.00          H
ATOM   6448 2HB  HIS A 578      -9.496   87.320  -0.407  1.00  0.00          H
ATOM   6449  HD2 HIS A 578      -8.418   88.779   1.444  1.00  0.00          H
ATOM   6450  HDl  HIS A 578      -5.828   86.722  -1.016  1.00  0.00          H
ATOM   6451  HE1 HIS A 578      -4.311   88.087   0.532  1.00  0.00          H
ATOM   6452  N   HIS A 579     -10.211   83.640  -1.458  1.00  0.00          N
ATOM   6453  CA  HIS A 579     -11.482   83.026  -1.836  1.00  0.00          C
ATOM   6454  C   HIS A 579     -11.547   81.576  -1.348  1.00  0.00          C
ATOM   6455  O   HIS A 579     -12.307   81.282  -0.426  1.00  0.00          O
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ATOM 6456 CB HIS A 579 -11.732 83.130 -3.351 1.00 0.00 C
ATOM 6457 CG HIS A 579 -12.230 84.473 -3.835 1.00 0.00 C
ATOM 6458 CD2 HIS A 579 -12.744 84.873 -5.045 1.00 0.00 C
ATOM 6459 ND1 HIS A 579 -12.262 85.613 -3.039 1.00 0.00 N
ATOM 6460 CE1 HIS A 579 -12.770 86.620 -3.766 1.00 0.00 C
ATOM 6461 NE2 HIS A 579 -13.099 86.214 -4.989 1.00 0.00 N
ATOM 6462 H HIS A 579 -9.392 83.100 -1.699 1.00 0.00 H
ATOM 6463 HA HIS A 579 -12.305 83.637 -1.465 1.00 0.00 H
ATOM 6464 1HB HIS A 579 -10.803 82.934 -3.887 1.00 0.00 H
ATOM 6465 2HB HIS A 579 -12.483 82.397 -3.647 1.00 0.00 H
ATOM 6466 HD2 HIS A 579 -12.819 84.167 -5.859 1.00 0.00 H
ATOM 6467 HD1 HIS A 579 -11.931 85.573 -2.085 1.00 0.00 H
ATOM 6468 HE1 HIS A 579 -12.864 87.605 -3.332 1.00 0.00 H
ATOM 6469 N TYR A 580 -10.799 80.662 -1.963 1.00 0.00 N
ATOM 6470 CA TYR A 580 -10.795 79.248 -1.613 1.00 0.00 C
ATOM 6471 C TYR A 580 -9.428 78.633 -1.905 1.00 0.00 C
ATOM 6472 O TYR A 580 -8.725 78.252 -0.980 1.00 0.00 O
ATOM 6473 CB TYR A 580 -11.895 78.510 -2.389 1.00 0.00 C
ATOM 6474 CG TYR A 580 -12.108 77.068 -1.959 1.00 0.00 C
ATOM 6475 CD1 TYR A 580 -11.545 75.996 -2.681 1.00 0.00 C
ATOM 6476 CD2 TYR A 580 -12.883 76.779 -0.820 1.00 0.00 C
ATOM 6477 CE1 TYR A 580 -11.763 74.664 -2.278 1.00 0.00 C
ATOM 6478 CE2 TYR A 580 -13.100 75.450 -0.418 1.00 0.00 C
ATOM 6479 CZ TYR A 580 -12.548 74.381 -1.145 1.00 0.00 C
ATOM 6480 OH TYR A 580 -12.778 73.093 -0.747 1.00 0.00 O
ATOM 6481 H TYR A 580 -10.188 80.935 -2.720 1.00 0.00 H
ATOM 6482 HA TYR A 580 -11.055 79.133 -0.560 1.00 0.00 H
ATOM 6483 HXT TYR A 580 -9.081 78.534 -2.923 1.00 0.00 H
ATOM 6484 1HB TYR A 580 -12.845 79.026 -2.252 1.00 0.00 H
ATOM 6485 2HB TYR A 580 -11.642 78.491 -3.449 1.00 0.00 H
ATOM 6486 HD1 TYR A 580 -10.940 76.191 -3.554 1.00 0.00 H
ATOM 6487 HD2 TYR A 580 -13.318 77.583 -0.245 1.00 0.00 H
ATOM 6488 HE1 TYR A 580 -11.327 73.851 -2.840 1.00 0.00 H
ATOM 6489 HE2 TYR A 580 -13.696 75.241 0.458 1.00 0.00 H
ATOM 6490 HH TYR A 580 -13.329 73.094 0.039 1.00 0.00 H
ENDMDL
END

Virtual docking

The virtual docking and scoring of a large number of molecules in a protein active site has proven to be a useful method for selecting molecules for screening. It has the potential to be less biased than pharmacophore-based methods, since the only assumption one must make is the region of the protein surface to target.

Starting from the structure reported in Appendix I, a virtual docking protocol (using Gold 3.0.1) has been applyied to a collection of 220000 compounds from the Asinex database that have been opportunely treated: the 2D structures have been initially converted into the corresponding 3D structures using the Cerius^2 software and the 3D compounds have been filtered on the basis of the followings criteria:

-Molecular weight $\leq$ 550

-Rotable bonds ≤ 10

-Number of H-bond acceptors ≤ 11

-Number of H-bond donors ≤ 6

-AlogP98 ≤ 6

-Lipinski rule of five violations ≤ 1

The resulting compounds have been submitted to conformational analysis (Cerius default parameters) and finally treated with OpenBabel using the following options: -d (to remove hydroges); -p (add hydrogens at physiological pH); -c (reset coordinates).

The resulting database of commercially available compounds has been automatically docked into the RNA binding site using the GOLD default parameters with the exception of the foliowings:

Population size = 100

Select_pressure = 1.1

N_island = 5

Max Ops = 100000

Niche_size = 2

Pt_crosswt = 95

Allele_mutatewt = 95

Migratewt = 10

Radius = 10

Origin = 6.38; -29.48; 26.06

Floodfill_atom_no = 2465

No_run = 10

Scoring function = chemscore

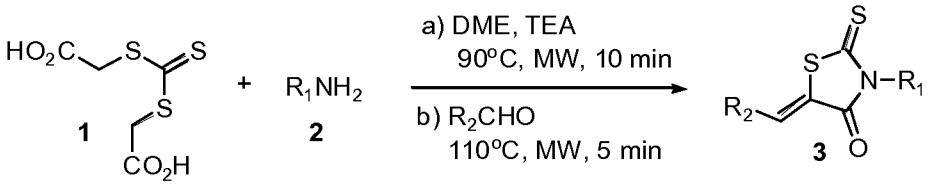
The 100 best ranking compounds (according to chemscore) were than re-docked into the RNA binding site increasing the number of runs up to 100. Visual inspection allowed to select the best candidate compounds defined by a chemscore value equal to or major than 25.

EXAMPLES

EXAMPLE 1

One-pot two-steps microwave-assisted synthesis of N-substituted 5-alkylidene-thiazol-4-ones.

General Procedure: To a solution of bis(carboxymethyl)trithiocarbonate **1** (1 eq.) in DME, TEA (1 eq.) and the amine **2** ($RiNH_2$, 1 eq.) were added. The reaction mixture was heated at 90°C under microwave irradiation for 10 min. After this time, the aldehyde (R_2CHO, 1 eq.) was added and the mixture was heated at 110°C under microwave irradiation for 5 min. The reaction mixture was evaporated to dryness and the residue was additioned with MeOH; the final rhodanine derivative was obtained as a pure precipitate upoun standing, isolated by filtration, washed with hexane and finally dried under high vacuum.



(Z)-5-(3-bromobenzylidene)-3-phenethyl-2-thioxothiazolidin-4-one (3a). Yellow solid. Mp 102-104 °C. ^1H NMR (400 MHz, $CDC1_3$) 7.56-7.49 (3H, m), δ 7.36-7.13 (7H, m), δ 4.30-4.26 (2H, t, *J* = 7.8 Hz), δ 2.96-2.92 (2H, t, *J* = 7.8 Hz) ppm. ^{13}C NMR (100 MHz, CDCI3) 192.5, 167.3, 137.3, 137.1, 135.3, 133.4, 133.1, 130.9, 130.7, 128.9, 126.9, 124.06, 123.0, 45.75, 32.93 ppm. Anal. Calcd for ($Ci_8Hi_4BrNOS_2$): C, 53.47; H, 3.49; N, 3.46. Found: C, 53.36; H, 3.40; N, 3.55.

(Z)-5-(3-bromobenzylidene)-3-benzyl-2-thioxothiazolidin-4-one (3b). Yellow solid. Mp 112-1 13 °C. ^1H NMR (400 MHz, $CDC1_3$) δ 7.55-7.47 (3H, m), δ 7.41-7.24 (7H, m), δ 5.25 (2H, s) ppm. ^{13}C NMR (100 MHz, $CDC1_3$) 192.5, 167.6, 135.3, 134.7, 133.5, 133.2, 131.2, 130.8, 129.0, 128.8, 128.6, 128.3, 124.7, 123.5, 47.6 ppm. Anal. Calcd for ($Ci_7Hi_2BrNOS_2$): C, 52.31; H, 3.10; N, 3.59. Found: C, 53.30; H, 3.21; N, 3.48.

(Z)-5-(3-bromobenzylidene)-3-ethynyl-2-thioxothiazolidin-4-one (3c). Orange solid. Mp 159-161 °C. ^1H NMR (400 MHz, CDCI3) δ 7.60 (1H, s), δ 7.55 (lH,s), δ 7.51-7.49 (1H, d, *J* = 7.7 Hz), δ 7.35-7.34 (1H, d, *J* = 7.7 Hz), δ 7.29-7.19 (1H, t, *J* = 7.7 Hz), δ 4.81-

4.80 (2H, d, J = 2.1 Hz), δ 2.19-2.18 (IH, t, J = 2.1 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) 191.2, 166.4, 135.2, 133.7, 133.6, 133.3, 133.2, 131.8, 131.6, 130.9, 130.7, 128.9, 128.7, 124.4, 123.5, 75.7, 72.3, 33.6 ppm. Anal. Calcd for ($C_{12}H_6BrNOS_2$):C, 44.45; H, 1.87; N, 4.32. Found: C, 44.37; H, 1.76; N, 4.42.

(Z)-5-(3-bromobenzylidene)-3-(2,2-dimethoxyethyl)-2-thioxothiazolidin-4-one (3d). Yellow solid. Mp 124-126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.52 (2H, m), δ 7.48-7.46 (IH, d, J = 7.8 Hz), δ 7.33-7.31 (IH, d, J = 7.8 Hz), δ 7.28-7.24 (IH, t, J = 7.8 Hz), δ 4.85-4.82 (IH, t, J = 5.6 Hz), 4.19-4.18 (2H, d, J = 5.6 Hz), 3.31 (6H, s) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) 193.0, 167.4, 135.3, 133.5, 133.2, 131.2, 130.7, 128.8, 124.5, 123.5, 99.3, 53.9, 45.0 ppm. Anal. Calcd for ($C_{14}H_{14}BrNO_3S_2$): C, 43.30; H, 3.63; N, 3.61. Found: C, 43.24; H, 3.60; N, 3.71.

(Z)-5-(3-bromobenzylidene)-3-butyl-2-thioxothiazolidin-4-one (3e). Yellow solid. Mp 113-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$) 7.51-7.45 (3H, m), 7.33-7.24 (2H, m), 4.05-4.02 (2H, t, J = 7.5 Hz), 1.61-1-59 (2H, m, J = 7.5 Hz), 1.32-1.29 (2H, m, J = 7.5 Hz), 0.90-0.87 (3H, t, J = 7.2 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) 192.7, 167.5, 135.4, 133.3, 133.2, 130.7, 128.7, 124.9, 123.4, 44.6, 29.0, 20.1, 13.7 ppm. Anal. Calcd for ($C_{14}H_{14}BrNOS_2$): C, 47.19; H, 3.96; N, 3.93. Found: C, 47.28; H, 3.88; N, 3.98.

(Z)-5-(3-methoxybenzylidene)-3-phenethyl-2-thioxothiazolidin-4-one (3f). Yellow solid. Mp 122-125. ^{1}H NMR (400 MHz, $CDCl_3$) 7.60 (IH, s), 7.34-7.18 (6H, m), 7.03-7.01 (IH, d), 6.92 (2H, s), 4.29-4.25 (2H, t, J = 7.9 Hz), 3.79 (3H, s), 2.96-2.92 (2H, t, J = 7.9 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) 193.1, 167.5, 160.1, 137.5, 134.6, 133.1, 130.4, 129.0, 128.9, 128.7, 128.6, 126.8, 123.2, 116.9, 115.2, 55.4, 45.7, 32.9 ppm. Anal. Calcd for ($C_{19}H_{17}NO_2S_2$): C, 64.20; H, 4.82; N, 3.94. Found: C, 64.31; H, 4.74; N, 3.85.

(Z)-5-((furan-2-yl)methylene)-3-phenethyl-2-thioxothiazolidin-4-one (3g). Orange solid. Mp 150-152 °C. ^{1}H NMR (400 MHz, $CDCl_3$) 7.63 (IH, s), 7.38 (IH, s), 7.3-7.1 (5H, m), 6.76 (IH, m), 6.52 (IH, m), 4.27-4.23 (2H, t, J = 7.9 Hz), 2.95-2.91 (2H, t, J = 7.9 Hz) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) 194.3, 167.3, 150.2, 147.0, 137.6, 129.0, 128.6, 126.8, 120.9, 118.6, 118.3, 113.5, 45.6, 33.0 ppm. Anal. Calcd for ($C_{16}H_{13}NO_2S_2$):. C, 60.93; H, 4.15; N, 4.44. Found: C, 60.89; H, 4.24; N, 4.35.

(Z)-3-phenethyl-5-((pyridin-3-yl)methylene)-2-thioxothiazolidin-4-one (3h). Yellow solid. Mp 138-140 °C. ¹H NMR (400 MHz, $CDC1_3$) 8.69 (1H, s), 8-57-8.56 (1H, d, J = 4.4 Hz), 7.70-7.68 (1H, d, J = 7.9 Hz), 7.59 (1H, s), 7.36-7.33 (1H, dd, J = 4.7 Hz, J = 7.9 Hz), 7.26-7.16 (5H, m), 4.28-4.24 (2H, t, J = 7.9), 2.95-2.91 (2H, t, J = 7.9 Hz) ppm. ^{13}C NMR (100 MHz, $CDC1_3$) 192.0, 167.1, 151.9, 150.8, 137.3, 136.3, 129.4, 128.9, 128.8, 128.7, 126.9, 125.5, 124.0, 45.8, 32.9 ppm. Anal. Calcd for ($C_{17}H_{14}N_2OS_2$): C, 62.55; H, 4.32; N, 8.58. Found: C, 62.58; H, 4.21; N, 8.50.

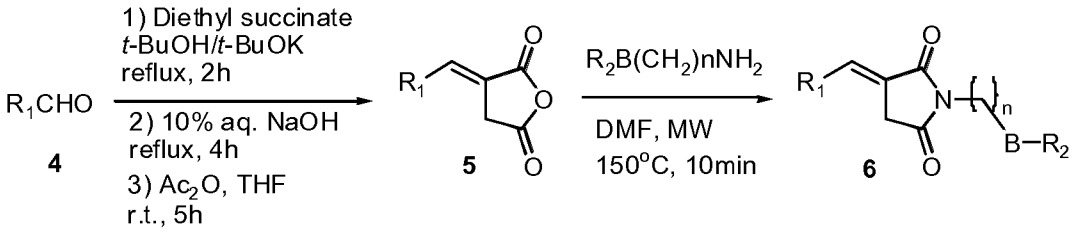
(Z)-5-((naphthalen-3-yl)methylene)-3-phenethyl-2-thioxothiazolidin-4-one (3i). Yellow solid. Mp 174-176 °C. ¹H NMR (400 MHz, $CDC1_3$) 7.90-7.79 (5H, m), 7.53-7.46 (3H, m), 7.29-7.19 (5H, m), 4.30-4.26 (2H, t, J = 7.9 Hz), 2.98-2.94 (2H, t, J = 7.9 Hz) ppm. ^{13}C NMR (100 MHz, $CDC1_3$) 193.1, 167.5, 137.6, 133.9, 133.2, 132.1, 130.8, 129.2, 129.0, 128.9, 128.7, 128.3, 127.8, 127.2, 126.8, 126.2, 45.7, 33.0 ppm. Anal. Calcd for ($C_{22}H_{17}NOS_2$): C, 70.37; H, 4.56; N, 3.73. Found: C, 70.28; H, 4.46; N, 3.70.

7V-(2-((Z)-5-(3-Bromobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)ethyl)-2-hydroxybenzamide (3j). Yield 69%. Yellow solid. ¹H NMR (400 MHz, DMSO-<¾): δ (ppm) 12.32 (s, 1H), 8.86 (t, J = 5.2 Hz, 1H), 7.80 (s, 1H), 7.71 (s, 1H), 7.63 (d, J = 7.9 Hz, 1H), 7.57-7.54 (m, 2H), 7.44 (t, J = 7.9 Hz, 1H), 7.30 (t, J = 7.7 Hz, 1H), 6.78 (t, J = 8.6 Hz, 2H), 4.20 (t, J = 5.2 Hz, 1H), 3.57 (q, J = 5.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSG-d_6): δ (ppm) 194.2, 170.2, 167.6, 160.7, 135.9, 133.9, 131.1, 129.0, 128.1, 124.8, 123.1, 115.4, 44.4, 36.7. MS (ESI) *mlz:* 462.9 [M-H]⁻. Anal. Calcd for ($Ci_9Hi_5BrN_20_3S_2$): C, 49.25; H, 3.26; N, 6.05. Found: C, 49.19; H, 3.34; N, 6.12.

7V-(2-((Z)-5-(3-Fluorobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)ethyl)-2-hydroxybenzamide (3k). Yield 62%. Yellow solid. ¹H NMR (400 MHz, DMSO-<¾): δ (ppm) 12.31 (1H, s), 8.85 (t, J = 4.6 Hz, 1H), 7.72 (1H, s), 7.58-7.50 (m, 2H), 7.45-7.37 (m, 2H), 7.31-7.29 (m, 2H), 6.80-6.76 (m, 2H), 4.20 (t, J = 4.5 Hz, 2H), 3.56 (q, J = 4.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSG-d_6): δ (ppm) 193.8, 169.8, 167.2, 164.8, 160.2, 135.4, 133.7, 131.7, 131.6, 130.8, 127.6, 126.0, 125.9, 124.3, 118.6, 117.4, 114.9, 43.9, 36.2. MS (ESI) *mlz:* 401.5 [M-H]⁻. Anal. Calcd for ($Ci_9Hi_5FN_20_3S_2$): C, 56.70; H, 3.76; N, 6.96. Found: C, 56.59; H, 3.83; N, 6.84.

EXAMPLE 2

Chemistry: Synthesis of pyrrolidine-2,5-dione derivatives



General Procedure for the synthesis of compounds 5: To a solution of potassium *tert*-butoxide, from 1.13 g (29 mmol, 1.2 eq) of potassium in 15 mL of *tert*-butyl alcohol at reflux was added 4.86 mL (29 mmol, 1.2 eq) of diethyl succinate in 2.8 mL of *tert*-butyl alcohol. A solution of the opportune benzaldehyde **4**(**1** eq) in 2.6 mL of tert-butyl alcohol was added dropwise and the resulting heterogeneous mixture was refluxed for 2h and then at r.t. overnight. After cooling, 30 mL of water was added and *tert*-butyl alcohol was removed by distillation. To this mixture a solution of 3.12 g (55.6 mmol, 2.3 eq) of KOH in 10 mL of water was added and mixture was heated at reflux for 4 h. The mixture was washed with Et_20. The acqueous layer was diluited with water and cone. HC1 was added up to pH 1. Then it was stirred 5 min. and it was extracted with Et_20, dried over Na_2S0_4 and then solvent was removed. The crude product was recrystallized from cyclohexane/hexane.

The latter intermediate (1.31 g, 5.87 mmol, 1 eq) was dissolved in THF, acetic anhydride (1.22 mL, 2.2 eq) was added and the resulting mixture stirred at room temperature for 5h. Then THF was removed and *tert*-butyl methylether (MTB-ether) was added to induce a more complete crystallization. The crystals are filtered, washed with MTB-ether and dried in vacuo.

General Procedure for the synthesis of compounds 6: Compounds with general structure **5** and the opportune amine (1 eq.) were suspended in a DMF (3 mL) and the mixture was heated with MW at 150°C for 10 min. Then water was added and the solution was extracted with CH_2C1_2. The organic layers were collected, washed with brine and dried over Na_2S0_4. The solvent was removed and residue was crystallized in EtOH to obtain the final product.

(E)-2-(3-fluorobenzylidene)succinic acid: ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.39 (s, 2H), δ 7.08-7.2 (m, 3H), δ 7.37-4.43 (m, 1H), δ 7.63 (m, 1H), δ 12.48 (br s, 2H) ppm. MS (ESI) *mlz:* 223 $[M-H]^-$. Anal. Calcd for (CnH_9F0_4): C, 58.93; H, 4.05. Found: C, 58.90; H, 3.98.

(E)-2-(3-bromobenzylidene)succinic acid: ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.26 (s, 2H), δ 7.32-7.33 (m, 2H), δ 7.48-7.53 (m, 2H), δ 7.62 (s, 1H), δ 12.55 (br s, 2H) ppm. MS (ESI) *mlz:* 284 $[M-H]^-$. Anal. Calcd for (CnH_9Br0_4): C, 46.34; H, 3.18. Found: C, 46.38; H, 3.28.

(E)-3-(3-fluorobenzylidene)-dihydrofuran-2,5-dione (5a): ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.93- 3.94 (d, 2H), δ 7.23-7.29 (m, 1H), δ 7.42-7.48 (m, 3H), 7.57 (s, 1H) ppm. MS (ESI) *mlz:* 205 $[M-H]^-$. Anal. Calcd for (CnH_7F0_3): C, 64.08; H, 3.42. Found: C, 64.12; H, 3.38.

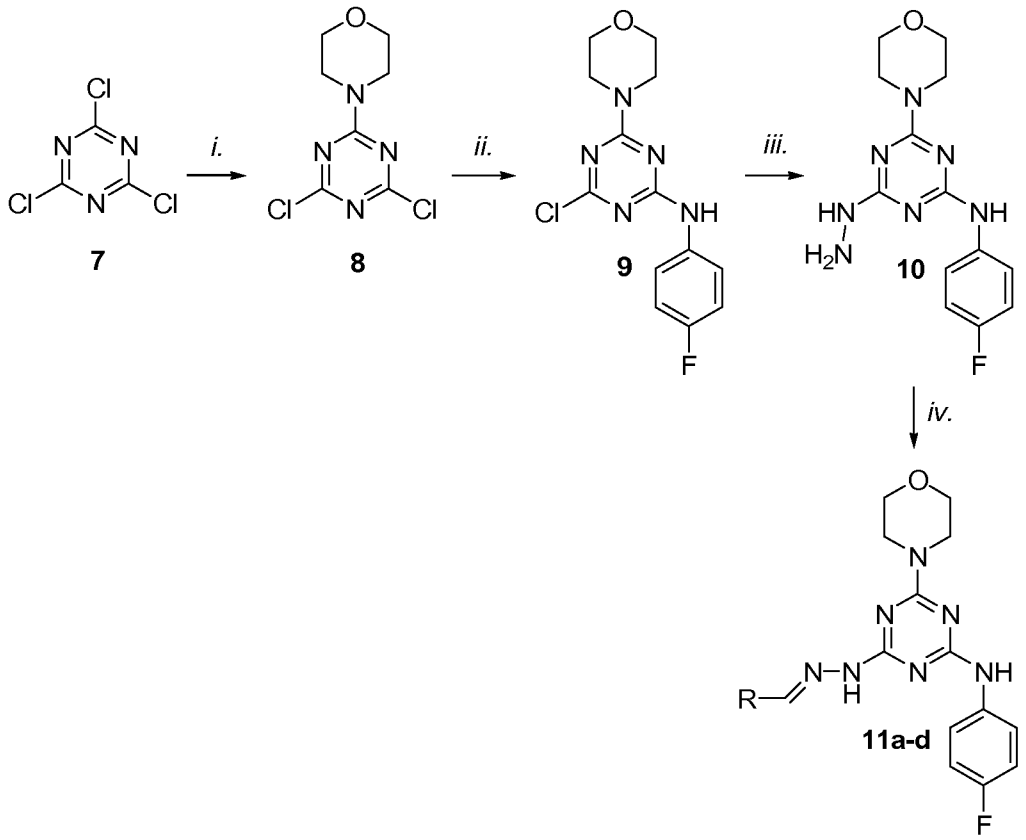
(E)-3-(3-bromobenzylidene)-dihydrofuran-2,5-dione (5b): ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.94-3.95 (d, 2H), δ 7.53-7.62 (m, 3H), δ 7.80 (s, 1H) ppm. MS (ESI) *mlz:* 266 $[M-H]^-$. Anal. Calcd for (CnH_7Br0_3): C, 49.47; H, 2.64. Found: C, 49.56; H, 2.66.

3-((E)-3-(3-fluorobenzylidene)-2,5-dioxopyrrolidin-l-yl)-N-(2-hydroxyphenyl)propanamide (6a): ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.59-2.65 (t, 2H, *J* = 6.3 Hz), δ 3.66 (s, 2H), δ 3.68-3.65 (t, 2H, *J* = 6.3 Hz), δ 6.63-6.70 (t, 1H, *J* = 7.2 Hz), δ 6.74-6.78 (d, 1H,), δ 6.82-6.88 (t, 1H, *J* = 7.2 Hz), 7.15-7.23 (d, 1H), 7.38-7.46 (m, 4H), 7.53-7.58 (d, 1H), 9.29 (s, 1H), 9.55 (s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) 34.1, 34.3, 35.4, 116.2, 116.8, 117.1, 119.3, 123.5, 125.3, 126.4, 126.8, 127.3, 131.1, 131.3, 136.9, 148.7, 161.5, 169.5, 170.7, 174.4 ppm. MS (ESI) *mlz:* 367 $[M-H]^-$. Anal. Calcd for ($C_{20}Hi_7FN_20_4$): C, 65.21; H, 4.65; N, 7.60. Found: C, 65.14; H, 4.72; N, 7.66.

3-((E)-3-(3-bromobenzylidene)-2,5-dioxopyrrolidin-l-yl)-N-(2-hydroxyphenyl)propanamide (6b): ^{1}H NMR (400 MHz, DMSO-d_6) δ 2.6 l(t, 2H, *J* = 7.1 Hz), δ 3.66 (s, 2H), δ 3.71 (t, 2H, *J* = 7.1 Hz), δ 6.67(t, 1H, *J* = 7.4 Hz), δ 6.76 (d, 1H, *J* = 7.6 Hz), 6.86 (t, 1H, *J* = 7.4 Hz), 7.31-7.41 (m, 2H), 7.53-7.60 (m, 3H), 7.77 (s, 1H), 9.28 (s, 1H), 9.54 (s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) 33.5, 33.6, 34.8, 115.7, 118.8,

122.2, 123.9, 124.6, 125.3, 126.9, 128.7, 130.3, 130.9, 132.3, 132.5, 136.4, 148.2, 168.2, 170.1, 173,8 ppm. MS (ESI) m/z:428.3 $[M-H]^-$. Anal. Calcd for ($C_{20}H_{17}BrN_{20}_4$): C, 55.96; H, 3.99; N, 6.53. Found: C, 55.88; H, 4.06; N, 6.46.

EXAMPLE 3



Reagents and conditions: *i.* DME, morpholine , 3h, -30°C; *ii.* CH_2C1_2, 4-F-aniline , 12h, reflux ; zzz.,CH_2C1_2, NH_2NH_2 H_20 , reflux, 12h; *iv.* toluene ,RCHO, 3h, reflux , Dean-Stark.

4-(4,6-dichloro-l,3,5-triazin-2-yl)morpholine (8): To a stirred solution of cyanuric chloride 7 (lg; 5.42mmol) in dimethoxy ethane (50 mL) at 30°C, morpholine (470.1 μL; 5.42 mmol) was added dropwise. The reaction mixture was vigorously stirred for 3h at -30°C then warmed up to room temperature and washed with HCl 3N, water, brine and finally dried over anhydrous Na_2S0_4. The product is obtained as a white solid used in the next step without further purification.

Yield = 79%; R_f (Et_20/Hex : 2:1) = 0.62; Mp 156.7-156.9 °C; 1H-NMR (400 MHz, CD_3OD): δ (ppm) 3.80(t, *J*=4.59 Hz, 4H); 3.66 (t, *J*=4.59 Hz, 4H); ^{13}C-NMR (100 MHz,

$CDCl_3$): δ (ppm) 170.44, 164.11, 66.37, 44.47; MS (ESI): *m/z* 235.1 $[M+H]^+$, 257.2 $[M+Na]^+$; Anal. Calcd for ($C_7H_8Cl_2N_4O$): C, 35.77; H, 3.43; N, 23.83. Found: C, 35.74; H, 3.38; N, 23.92.

4-chloro-N-(4-fluorophenyl)-6-morpholino-l,3,5-triazin-2-amine (9): To a stirred solution of compound **8** (650mg, 2.76 mmol) in dichloromethane, 4-fluoro aniline (310.81 μL , 2.71 mmol) was added. The reaction mixture was refluxed for 12h and then washed with HC1 3N, water, brine and finally dried over anhydrous Na_2SO_4. The organic phase was evaporated to dryness and the white residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether the final compound precipitated as a white solid and was collected by filtration.

Yield = 90%; R_f (Et_2O:Hex 2:1) = 0.51; Mp 170-172 °C; 1H-NMR (400 MHz, $CDCl_3$): δ (ppm) 7.38(q, J= 8.60 ,2H); 6.97 (t, J=8.63 Hz, 2H); 3.78 (brs, 2H); 3.72 (brs, 2H); 3.67-3.66 (m, 4H); MS (ESI): *m/z* 310.7 $[M+H]^+$; 332.6 $[M+Na]^+$; Anal. Calcd for ($C_{13}H_{13}ClFN_5O$): C, 50.41; H, 4.23; N, 22.61. Found: C, 50.35; H, 4.19; N, 22.69.

N-(4-fluorophenyl)-4-hydrazinyl-6-morpholino-l,3,5-triazin-2-amine (10): To a solution of **9** (900 mg; 2.69 mmol) in dichloromethane, hydrazine (544.2 μL, 10.76 mmol) was added and the resulting mixture was refluxed for 12 h. After cooling down to room temperature, the mixture was washed with water, brine and finally dried over anhydrous Na_2SO_4. The organic phase was evaporated to dryness and the residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether the final compound precipitated as a white solid and was collected by filtration.

Yield = 70%; R_f (CH_2Cl_2:CH_3OH 95:5) = 0.54; MS (ESI): *m/z* 306 $[M+H]^+$;Anal. Calcd for ($C_{13}H_{16}FN_7O$): C, 51.14; H, 5.28; N, 32.11. Found: C, 51.07; H, 5.33; N, 32.02.

Synthesis of the final compounds lla-c.

General procedure: To a stirred solution of **10** in toluene, the opportune aldehyde (2 eq) was added and the resuting mixture was refluxed for 3 h using a Dean-Stark apparatus for azeotropical removal of water. The reaction mixture was evaporated to dryness and the resulting residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether the final compound precipitated and collected by filtration.

(E)-N-(4-fluorophenyl)-4-morpholino-6-(2-(naphthalen-l-ylmethylene)hydrazinyl)-l,3,5-triazin-2-amine (11a): Yield = 80%; R_f (CH_2Cl_2:MeOH 95:5) = 0.53; Mp 220.0-

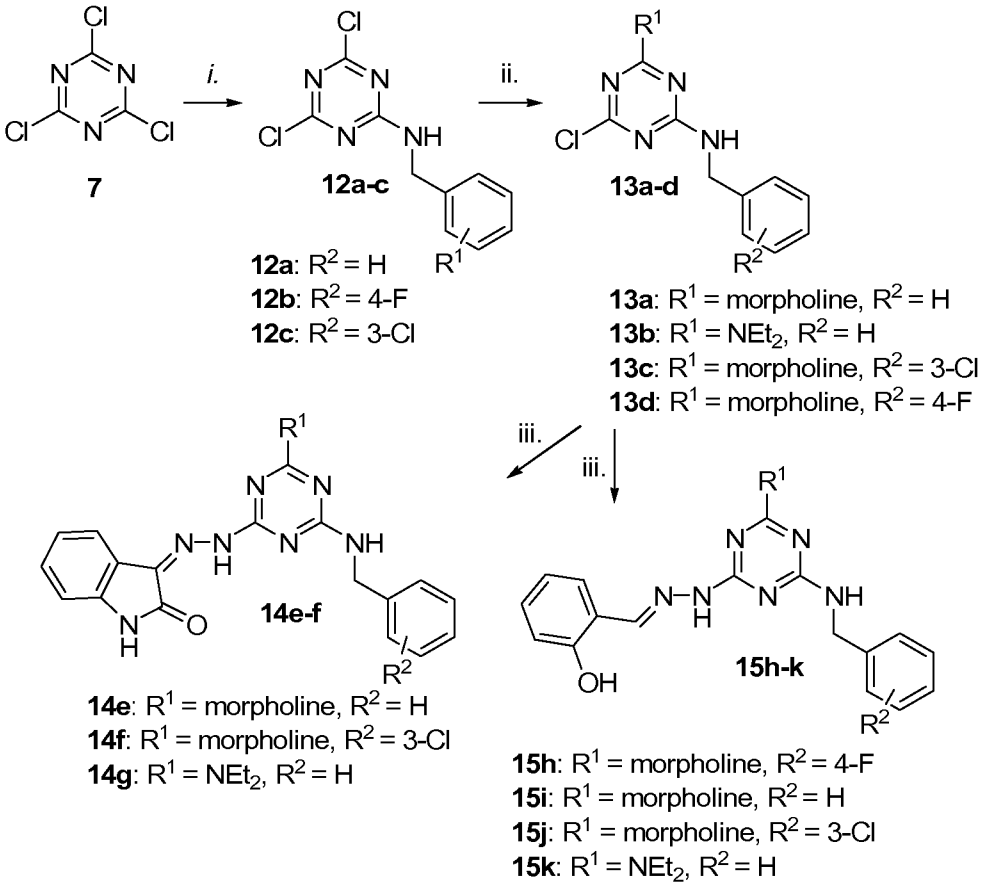
220.4 °C; 1H-NMR (400 MHz, $CDC1_3$): δ (ppm) 8.62 (1H); 8.47 (1H); 7.91-7.81 (m, 3H); 7.53-7.49 (m, 5H); 6.99 (t, J=8.4; 3H); 3.82 (s, 4H); 3.76 (s, 4H); ^{13}C-NMR (100 MHz, $CDC1_3$): δ (ppm) 165.85, 161.14, 156.33, 142.59, 133.83, 128.77, 127.56, 127.03, 126.82, 126.26, 121.81, 115.14, 77.62, 76.99, 76.35, 66.75, 43.80; MS (ESI): *m/z* 444.2 $[M+H]^+$; Anal. Calcd for ($C_{24}H_{22}FN_7O$): C, 65.00; H, 5.00; N, 22.11. Found: C, 65.06; H, 5.10; N, 22.02.

(E)-N-(4-fluorophenyl)-4-morpholino-6-(2-(naphthalen-2-ylmethylene)hydrazinyl)-l,3,5-triazin-2-amine (lib): Yield = 83%; R_f (CH_2Cl_2:MeOH 95:5) = 0.62; Mp 225-226 °C; 1H-NMR (400 MHz, $CDC1_3$): δ (ppm) 10.95 (brs ,1H); 8.22(s,lH); 7.93-7.83 (m, 6H); 7.46-7.44 (m,2H); 7.05(t, J=8.5; 2H); 3.68 (s, 4H); 3.58(s,4H); ^{13}C-NMR (100, MHz, $CDC1_3$): δ (ppm) 165.26, 164.62, 158.94, 156.57, 142.89, 137.18, 133.80, 133.48, 133.44, 133.28, 128.83, 128.59, 128.21, 128.08, 127.14, 122.92, 121.76, 115.41, 115.19, 66.49, 43.90; MS (ESI): *m/z* 444.5 $[M+H]^+$; Anal. Calcd for ($C_{24}H_{22}FN_7O$): C, 65.00; H, 5.00; N, 22.11. Found: C, 65.05; H, 5.09; N, 22.14.

(E)-4-(2-(2,6-difluorobenzylidene)hydrazinyl)-N-(4-fluorophenyl)-6-morpholino-l,3,5-triazin-2-amine (11c): Yield = 85%; R_f (CH_2Cl_2:MeOH: 95:5) = 0.65; Mp 155.5-156 °C; 1H-NMR ($CDC1_3$): δ (ppm) 8.61 (s, 1H); 7.95 (s, 1H); 7.45 (brs, 3H); 7.23-7.10 (m, 1H); 6.96-6.91 (t, J=8.5 Hz ,1H); 6.88-6.83 (t, J=8.5 Hz, 2H); 3.75 (s, 4H); 3.68 (s, 4H); ^{13}C-NMR ($CDC1_3$): δ (ppm)163.60, 163.47, 161.16, 158.60, 156.35, 133.33, 130.48, 121.75. 115.59, 115.15, 112.07, 111.68, 77.63, 77.20, 76.36, 66.70, 43.83; MS (ESI): *m/z* 430 $[M+H]^+$; Anal. Calcd for ($C_{2o}Hi_8F_3N_70$): C, 55.94; H, 4.23; N, 22.83. Found: C, 55.96; H, 4.29; N, 22.88

(£)-2-((2-(4-(4-Fluorophenylamino)-6-morpholino-l,3,5-triazin-2-yl)hydrazono) methyl)phenol (lid). Mp 234 °C. H NMR (400 MHz, $CDCl_3$-*d*): δ (ppm) 11.37 (brs, 1H), 7.84 (s, 1H), 7.42 (brs, 1H), 7.22-7.19 (m, 1H), 7.09-7.07 (m, 1H), 6.98-6.93 (m, 3H), 6.84-6.80 (m, 1H), 3.77-3.68 (m, 8H). MS (ESI) *m/z*: 410.4 $[M+H]^+$; 432 $[M+Na]^+$. Anal. Calcd for ($C_{20}H_{20}FN_7O_2$): C, 58.67; H, 4.92; N, 23.95. Found: C, 58.71; H, 4.86; N, 23.99.

EXAMPLE 4



Reagents and conditions: *i.* DME, -30 °C, R^2BnNH_2, 3 h; *ii.* CH_2Cl_2, R^H, r.t., 12 h; *Hi.* a) CH_2Cl_2, $NH_2NH_2 H_20$, reflux, 12 h; b) toluene, isatin (for **14e-f)** or salicylaldehyde (for **14h-k),** 3 h, reflux, Dean-Stark.

General procedure for the synthesis of compound 12a-c. To a stirred solution of cyanuric chloride 7(lg, 5.42 mmol) in dimethoxyethane (35 mL) at -30 °C, the opportune benzylamine (1 eq) was added dropwise. The reaction mixture was vigorously stirred for 3 h at -30 °C then, warmed up to room temperature and washed with 3N HCl, water, brine and finally dried over anhydrous Na_2S0_4.The organic phase was evaporated to dryness and the white residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether, the final compounds precipitated and were collected by filtration.

7V-Benzyl-4,6-dichloro-l,3,5-triazin-2-amine (12a). Yield 85%. ¹H NMR (200 MHz, $COCl_3$-*d*): δ (ppm) 7.30-7.26 (m, 5H), 4.48 (m, 2H), MS (ESI): *m/z:* 256.1 $[M+H]^+$. Anal. Calcd for ($Ci_0H_9Cl_2N_4$): C, 47.08; H, 3.16; N, 21.96. Found: C, 47.02; H, 3.21; N, 22.04.

4,6-Dichloro-7V-(4-fluorobenzyl)-l,3,5-triazin-2-amine (12b): Yield 75%. Mp 151.0-151.5 °C. ¹H NMR (400 MHz, *CO_3OO-d_4):* δ (ppm) 7.23-7.19 (m, 2H), 6.98 (t, *J* = 8.48 , 2H), 6.19 (brs,lH). MS (ESI) *m/z:* 274.1 $[M+H]^+$. Anal. Calcd for ($C_{10}H_7CI_2FN_4$): C, 43.98; H, 2.58; N, 20.52. Found: C, 43.88; H, 2.62; N, 20.59.

4,6-Dichloro-7V-(3-chlorobenzyl)-l,3,5-triazin-2-amine (12c): Yield 78%. Mp 149 °C. ¹H NMR (400 MHz, *CO_3OO-d_4):* δ (ppm) 7.23-7.19 (m, 3H), 7.13-7.10 (m, 1H), 6.58 (brs, 1H), 4.60 (d, *J* = 6.29 , 2H). ^{13}C NMR (100 MHz, *$COCl_3$-d)*: δ (ppm)169.95, 165.98, 138.48, 134.76, 130.18, 128.24, 127.70, 125.73, 44.68. MS (ESI) *m/z:* 289.5 $[M+H]^+$; 311.5 $[M+Na]^+$. Anal. Calcd for ($C_{10}H_7CI_3N_4$): C, 41.48; H, 2.44; N, 19.35. Found: C, 41.45; H, 2.38; N, 19.36.

General procedure for the synthesis of compounds 13a-d. To a suspension of the opportune intermediate **12a-c** (1 eq) in dichloromethane, the opportune amine (2 eq) was added dropwise. The reaction mixture was stirred at room temperature for 12 h and then washed with 3N HCl, water, brine and finally dried over anhydrous Na_2S0_4. The organic phase was evaporated to dryness and the white residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether the final compounds precipitated and were collected by filtration.

7V-Benzyl-4-chloro-6-morpholino-l,3,5-triazin-2-amine (13a). Yield 67%. ¹H NMR (200 MHz, *$CDCl_3$-d)*: δ (ppm) 7.28-7.25 (m, 5H), 7.07 (brs, 1H), 4.58 (d, *J* = 6 Hz, 2H), 3.74-3.65 (m, 8H). MS (ESI): *m/z* 306.8 $[M+H]^+$. Anal. Calcd for ($Ci_4Hi_6ClN_50$): C, 54.99; H, 5.27; N, 22.90. Found: C, 55.05; H, 5.25; N, 22.87.

7V2-Benzyl-6-chloro-7V4^V4-diethyl-l,3,5-triazine-2,4-diamine (13b): Yield 75%. ¹H NMR (200 MHz, *CDCh-d):* δ (ppm) 7.29-7.24 (m, 5H), 6.06 (brs, 1H), 4.57 (s, 2H), 3.55-3.48 (m, 4H), 1.16-1.07 (m, 6H). MS (ESI) *m/z*: 292.8 $[M+H]^+$. Anal. Calcd for ($Ci_4Hi_5Cl_2N_5$): C, 57.63; H, 6.22; N, 24.00. Found: C, 57.60; H, 6.16; N, 24.08.

4-Chloro-7V-(3-chlorobenzyl)-6-morpholino-l,3,5-triazin-2-amine (13c): Yield 85%. Mp 168-168.5 °C. ¹H NMR (400 MHz, *CD_3OD-d_4):* δ (ppm) 7.72 (s, 1H), 7.19-7.16 (m, 2H), 6.67 (brs, 1H), 4.54-4.49 (m, 2H), 3.72-3.61 (m, 8H). ^{13}C NMR (100 MHz, *COCh-d):* δ (ppm) 165.46, 164.34, 163.10, 144.97, 134.07, 129.34, 128.90, 128.82, 115.42, 115.21, 66.54, 66.37, 44.03, 43.79. MS (ESI) *m/z:* 340.1 $[M+H]^+$. Anal. Calcd for ($Ci_4Hi_5Cl_2N_5$): C, 49.43; H, 4.44; N, 20.59. Found: C, 49.40; H, 4.46; N, 20.51.

4-Chloro-7V-(4-fluorobenzyl)-6-morpholino-l,3,5-triazin-2-amine (13d): Yield 95%. Mp 192 °C. ¹H NMR (400 MHz, *CO_3OO-d_4):* δ (ppm) 7.23-7.17(m, 2H), 6.95 (t, *J* = 8.43, 2H), 6.00 (brs, 1H), 4.52-4.47 (m, 2H), 3.72 (s, 4H), 3.62 (s, 4H). MS (ESI) *m/z:* 324.7 $[M+H]^+$. Anal. Calcd for ($C_{14}H_{15}C1FN_50$): C, 51.94; H, 4.67; N, 21.63. Found: C, 51.88; H, 4.74; N, 21.60.

General procedure for the synthesis of compounds 14e-g and 15h-k. To a solution of the opportune intermediate **13a-d** (1 eq) in dichloromethane, hydrazine (4 eq) was added and the resulting mixture was refluxed for 12 h. After cooling down to room temperature, the mixture was washed with water, brine and finally dried over anhydrous Na_2S0_4. The organic phase was evaporated to dryness, the residue was dissolved in toluene and reacted with the opportune aldehyde (2 eq). The reaction mixture was refluxed for 3 h using a Dean-Stark apparatus for azeotropical removal of water. The reaction mixture was evaporated to dryness and the resulting residue was dissolved with the minimum amount of dichloromethane; by addition of petroleum ether the desired compounds **14e-g** and **15h-k** precipitated and were collected by filtration.

(£)-3-((2-(4-(Benzylamino)-6-morpholino)-l,3,5-triazin-2-yl)hydrazono)indolin-2-one (14e). Yield 80%. ¹H NMR (400 MHz, *COCh-d):* δ (ppm), 12.39 (s, 1H), 8.87 (s, 1H), 7.60-7.58 (m, 1H), 7.34-7-30 (m, 6H), 6.96-6.95 (m, 1H), 6.83-6.81 (m, 1H), 6.15 (brs, 1H), 4.64 (s, 2H), 3.60-3.57 (m, 4H), 1.26-1.12 (m, 6H). ^{13}C NMR *($COCl_3$-d)*: δ (ppm) 164.42, 163.26, 141.17, 139.76, 138.15, 137.82, 129.86, 127.88, 126.80, 126.38, 122.17, 120.82, 120.17, 110.26, 43,99, 40.93, 12.03. MS (ESI) *m/z:* 431.5 $[M+H]^+$. Anal. Calcd for ($C2_2H_{22}N_802$): C, 61.38; H, 5.15; N, 26.03. Found: C, 61.34; H, 5.21; N, 26.09.

(Z)-3-(2-(4-(3-Chlorobenzylamino)-6-morpholino-l,3,5-triazin-2-yl)hydrazono)indolin-2-one (14f). Yield 71%. Mp 144-144.5 °C. ¹H NMR (400 MHz, *CO_3OO-d_4):* δ (ppm) 12.39 (s, 1H), 8.15 (s, 1H), 7.62 (d, *J* = 6.80, 1H), 7.26 (s, 1H), 7.16 (m, 4H), 7.00-6.90 (m, 1H), 6.77 (d, *J* = 7.82), 4.53 (s, 2H), 3.75 (s , 4H), 3.65 (s, 4H). ^{13}C NMR (100 MHz, *COCh-d):* δ (ppm) 165.08, 164.26, 163.10, 141.13, 139.84, 134.33, 132.42, 130.15, 129.75, 127.68, 127.32, 125.50, 122.93, 121.33, 120.88, 110.47, 66.76, 44.40, 43.77. MS (ESI) *m/z:* 465.9 $[M+H]^+$. Anal. Calcd for ($C_{22}H_2iClN_80_2$): C, 56.84; H, 4.55; N, 24.10. Found: C, 56.88; H, 4.47; N, 24.11.

(£)-3-(2-(4-(benzylamino)-6-(diethylamino)-l,3,5-triazin-2-yl)hydrazono)indolin-2-one (14g) Yield 78%. ¹H NMR (400 MHz, *COCh-d):* δ (ppm) 11.52 (s, 1H), 7.92 (s, 2H),

7.33 (s, 3H), 7.18-7.17 (m, 1H), 7.01-6.99 (m, 1H), 6.91-6.87 (m, 1H), 4.63 (s, 2H), 3.82-3.73 (m, 8H). MS (ESI) *m/z: All .5* $[M+H]^+$. Anal. Calcd for ($C_{22}H_{24}N_8O$): C, 63.45; H, 5.81; N, 26.90. Found: C, 63.53; H, 5.88; N, 26.81.

(£)-2-((2-(4-(4-fluorobenzylamino)-6-morpholino-l,3,5-triazin-2-yl)hydrazono)methyl)phenol (15h). Yield 87%. Mp 114-1 14.5 °C. ¹H NMR (400 MHz, **CD_3OD-*d_4*):** δ (ppm) 11.48 (s, 1H), 7.77 (s, 1H), 7.19 (s, 3H), 7.02 (s, 1H), 6.91 (s, 3H), 6.80 (t, *J* = 6.63 Hz, 1H), 4.47 (s, 2H), 3.74 (s, 4H), 3.65 (s, 4H). ^{13}C NMR (100 MHz, *$CDCl_3$-d)*: δ (ppm) 165.07, 163.85, 163.31, 160.82, 158.07, 143.85, 134.75, 130.81, 129.78, 129.19, 119.18, 118.15, 117.02, 115.51, 115.30, 66.81, 44.13, 43.72. MS (ESI) *m/z:* 424.4 $[M+H]^+$; 446.4 $[M+Na]^+$. Anal. Calcd for (C21H22FN7O2): C, 59.57; H, 5.24; N, 23.15. Found: C, 59.56; H, 5.06; N, 23.14.

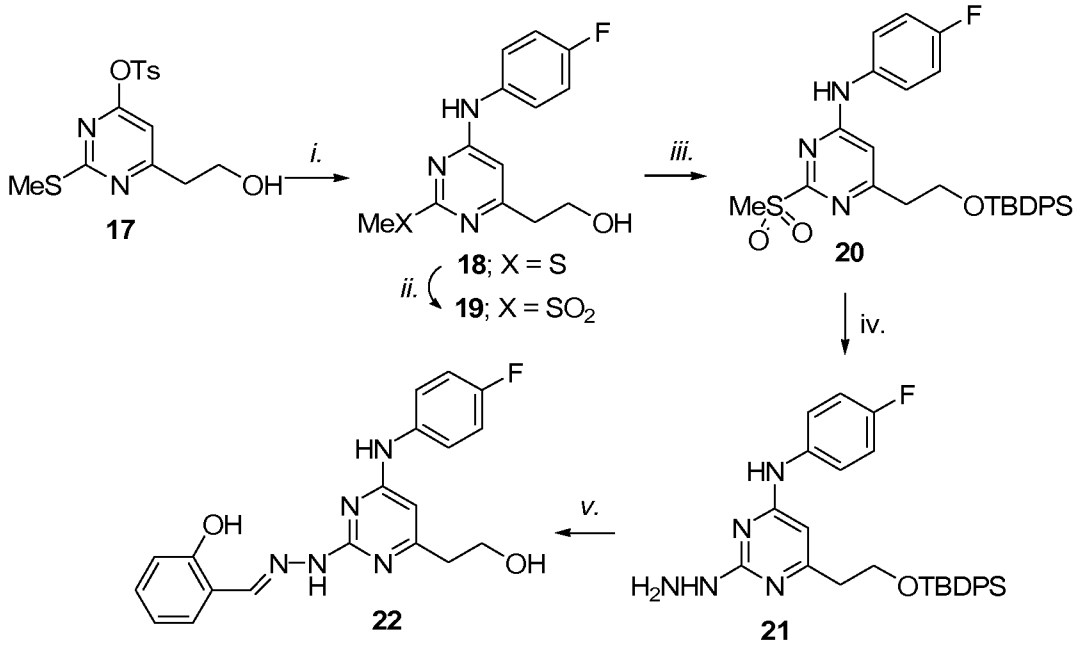
(£)-2-((2-(4-(Benzylamino)-6-morpholino-l,3,5-triazin-2-yl)hydrazono)methyl) phenol (15i). Yield 74 %. ¹H NMR (400 MHz, *CDCh-d):* δ (ppm) 12.47 (s, 1H), 9.27 (s, 1H), 7.51-7.49 (m, 1H), 7.32-7.23 (m, 5H), 7.15-7.13 (m, 1H), 7.05-7.01 (m, 1H), 6.90-6.79 (m, 1H), 6.48 (brs, 1H), 4.64 (s, 2H), 3.84-3.72 (m, 8H). ^{13}C NMR *{$CDCl_3$-d):* δ (ppm) 166.07, 165.05, 164.13, 163.32, 139.96, 138.83, 132.51, 129.99, 128.40, 127.41, 127.10, 122.74, 121.16, 120.72, 110.48, 66.70, 44.88, 43.68. MS (ESI) *m/z:* 406.5 $[M+H]^+$. Anal. Calcd for (C21H23N7O2): C, 62.21; H, 5.72; N, 24.18. Found: C, 62.26; H, 5.64; N, 24.15.

(£)-2-((2-(4-(3-chlorobenzylamino)-6-morpholino-l,3,5-triazin-2-yl)hydrazono)methyl)phenol (15j). Yield 82%. Mp 163.5-164 °C. ¹H NMR (400 MHz, CD_3OD-^): δ (ppm) 11.51 (s, 1H), 7.83 (s, 1H), 7.29-7.07 (m, 3H), 6.96 (d, *J* = 8.2, 1H), 6.84 (t, *J* = 7.4, 3H), 4.54 (d, *J* = 4.9 Hz, 2H), 3.77 (s, 4H), 3.71 (s, 4H). ^{13}C NMR (100 Hz, *COCh-d):* δ (ppm) 164.84, 158.00, 143.93, 141.09, 134.32, 130.75, 129.76, 127.57, 127.34, 125.48, 119.10, 118.04, 116.93, 66.68, 44.16, 43.66. MS (ESI) *m/z:* 440.9 $[M+H]^+$; 462.9 $[M+Na]^+$. Anal. Calcd for (C21H22CIN7O2): C, 57.34; H, 5.04; N, 22.29. Found: C, 57.37; H, 5.12; N, 22.21.

(£)-2-((2-(4-(benzylamino)-6-(diethylamino)-l,3,5-triazin-2-yl)hydrazono)methyl)phenol (15k). Yield 85%. ¹H NMR (400 MHz, *COCh-d):* δ (ppm) 11.54 (brs, 1H), 7.86 (s, 1H), 7.31-7.19 (m, 6H), 7.10-7.08 (m, 1H), 6.97-6.95 (m, 1H), 6.85-6.82 (m, 1H), 5.24 (brs, 1H), 4.59-4.57 (m, 2H), 3.56 (m, 4H), 1.18-1.1 1 (m, 6H). MS

(ESI) *m/z*: 392.5 $[M+H]^+$. Anal. Calcd for ($C_{21}H_{25}N_7O$): C, 64.43; H, 6.44; N, 25.05. Found: C, 64.38; H, 6.48; N, 25.00.

EXAMPLE 5



Reagents and conditions: *i.* 4-Fluoroaniline, DME, MW, 150°C, 5 min; *ii.* Oxone, H_20/MeOH/THF; *iii.* .TBDPSC1, DMF, imidazole, MW, 100°C, 5 min; *iv.* hydrazine monohydrate,, DME, 120°C, 5 min; v. a) salicylaldehyde, toluene, molecular sieves, reflux, overnight; b) Et_3N-3HF, THF, r.t., overnight.

2-(6-(4-Fluorophenylamino)-2-(methylthio)pyrimidin-4-yl)ethanol (18). A mixture of **17** (0.28 mmol) and 4-fluoroaniline (1.12 mmol) in dimethoxyethane was irradiated under microwave at 150 °C for 5 min. The reaction mixture was then concentrated under reduced pressure, diluted with EtOAc and washed with water, dried and purified by flash chromatography (DCM/EtOAc: 1/1) to get the desired product **18.**

Yield 80%. ʜ NMR (400 MHz, *COCl₃-d):* δ (ppm) 7.3 (m, 2H), 7.1 (t, 2H), 6.62 (s, 1H), 6.1 (s, 1H), 3.95 (t, *J* = 8 Hz, 2H), 2.75 (t, *J* = 8 Hz, 2H), 2.5 (s, 3H). ^{13}C NMR (50 MHz, CD30D-<¾): δ (ppm) 172.75, 167.07, 162.66, 162.06, 157.88, 136.88, 123.84, 123.69, 116.42, 115.97, 101.83, 61.56, 40.98, 14.16. MS (ESI) *m/z:* 280.3 $[M+H]^+$. Anal. Calcd for ($C_{13}H_{14}FN_3OS$): C, 55.90; H, 5.05; N, 15.04. Found: C, 55.95; H, 5.12; N, 15.08.

2-(6-(4-Fluorophenylamino)-2-(methylsulfonyl)pyrimidin-4-yl)ethanol (19). Compound **18** (0.448 mmol) was dissolved in a 1:1 mixture of MeOH and H_20 (6 mL); Oxone (0.896 mmol) in 3 mL of water was added portionwise and the mixture was then stirred overnight at r.t.. The crude mixture was concentrated under reduced pressure, neutralized with $NaHC0_3$ solution and washed with EtOAc. The organic extracts were collected, dried over Na_2S0_4, and then evaporated under reduced pressure. The crude residue was purified by flash chromatography (CH_2Cl_2:AcOEt 1:1) to give the desired product **19.**

Yield = 71%. ^{1}H NMR (200 MHz, $CDCl_3$-*d*): δ (ppm) 7.55 (br, 1H), 7.35 (m, 2H), 7.1 (m, 2H), 6.55 (s, 1H), 3.95 (t, ***J*** = 8 Hz, 2H), 3.3 (s, 3H), 2.85 (t, ***J*** = 8 Hz, 3H). ^{13}C NMR (50 MHz, ***CO$_3$OO-d$_4$):*** δ (ppm) 168.72, 166.44, 163.15, 162.83, 158.83, 136.07, 124.13, 116.78, 116.33, 108.58, 61.11, 41.14, 39.31. MS (ESI) ***m/z***: 312.3 $[M+H]^+$. Anal. Calcd for ($Ci_3Hi_4FN_30_3S$): C, 50.15; H, 4.53; N, 13.50. Found: C, 50.18; H, 4.47; N, 13.59.

6-(2-(terf-Butyldiphenylsilyloxy)ethyl)-*N*-(4-fluorophenyl)-2(methylsulfonyl)pyrimidin-4-amine (20). Compound **19** (0.16 mmol) and ***tert***-butyldiphenylsilylchloride (0.16 mmol) were dissolved in dry DMF and the mixture was irradiated under microwave at 100 °C for 5 min. The reaction mixture was diluted with EtOAc, washed several times with water, brine, dried over Na_2S0_4. The crude material was purified by flash chromatography (DCM/EtOAc: 9/1) to give the desired product **20.**

Yield = 80%. ^{1}H NMR (200 MHz, C***OC***l$_3$-***d):*** δ (ppm) 7.55 (m, 4H), 7.40 (m, 6H), 7.25 (m, 2H), 7.05 (m, 2H), 6.60 (s, 1H), 4.00 (t, ***J*** = 8 Hz, 2H), 3.20 (s, 3H), 2.75 (t, ***J*** = 8 Hz, 2H), 0.95 (s, 9H). ^{13}C NMR (50 MHz, ***C***D***C***l$_3$-***d):*** δ (ppm) 168.95, 165.20, 163.10, 162.16, 158.10, 135.35, 133.18, 129.74, 127.68, 125.61, 125.46, 116.76, 116.30, 105.22, 61.98, 40.65, 38.79, 29.63, 26.67. MS (ESI) ***m/z:*** 550.7 $[M+H]^+$. Anal. Calcd for ($C_{29}H_{32}FN_30_3SSi$): C, 63.36; H, 5.87; N, 7.64. Found: C, 63.43; H, 5.80; N, 7.60.

6-(2-(tei"i-Butyldiphenylsilyloxy)ethyl)-7V-(4-fluorophenyl)-2-hydrazinylpyrimidin-4-amine (21). Compound **20** (0.2 mmol) was dissolved in dimethoxyethane (2 mL) and the resulting mixture was irradiated under microwave at 120 °C for 5 min. The solvent was evaporated under reduced pressure and the remaining crude material was purified by flash chromatography (DCM/MeOH: 9.5/0.5) to give the desired product **21.**

Yield = 90%. ^{1}H NMR (400 MHz, CD***CY-d):*** δ (ppm) 7.50 (d, ***J*** = 4 Hz, 4H), 7.27 (m, 6H), 7.2 (m, 2H), 6.95 (t, ***J*** = 8 Hz, 2H), 5.87 (s, 1H); 3.89 (t, ***J*** = 8 Hz, 2H), 2.61 (t, ***J*** = 8 Hz, 2H), 0.91 (s, 9H). ^{13}C NMR (100 MHz, ***C***D***C***l$_3$-***d):*** δ (ppm) 161.98, 161.02, 158.58,

135.43, 134.82, 134.50, 133.65, 129.62, 127.75, 127.60, 127.53, 124.81, 124.73, 116.12, 115.89, 95.26, 62.54, 40.77, 29.70, 26.81. MS (ESI) *m/z:* 502.7 $[M+H]^+$. Anal. Calcd for ($C_{28}H_{32}FN_5OSi$): C, 67.04; H, 6.43; N, 13.96. Found: C, 67.12; H, 6.40; N, 13.94.

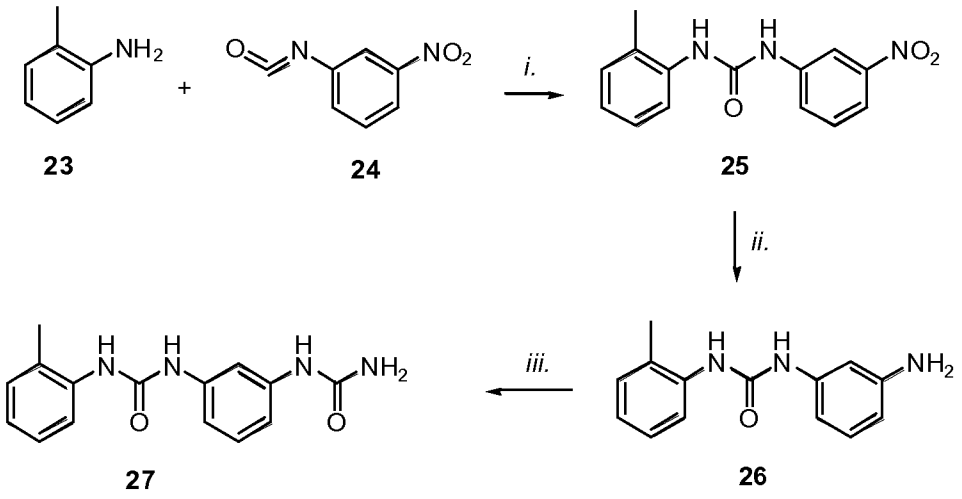
2-((2-(4-(2-(tei"i-Butyldiphenylsilyloxy)ethyl)-6-(4-fluorophenylamino)pyrimidin-2-yl) hydrazono)methyl)phenol. Compound **21** (0.046 mmol) and salicylaldehyde (0.046 mmol) were dissolved in dry toluene containing molecular sieves and the mixture was refluxed for 2 h, then it was cooled to r.t., concentrated under reduced pressure and purified by flash chromatography (DCM/EtOAc: 9/1) to give the desired product.

Yield = 54%. ^1H NMR (200 MHz, $CDCl_3$-*d):* δ (ppm) 8.05 (s, 1H), 7.55 (d, *J* = 4 Hz, 4H), 6.7-7.4 (m, 14H), 5.9 (s, 1H), 3.9 (t, *J* = 8 Hz, 2H), 2.7 (t, *J* = 8 Hz, 2H), 0.95 (s, 9H). ^{13}C NMR (50 MHz, *COCh-d):* δ (ppm) 166.78, 162.35, 162.22, 158.34, 157.97, 143.825, 135.50, 133.94, 133.88, 133.47, 130.50, 129.78, 129.61, 127.63, 124.58, 124.52, 119.13, 118.39, 116.92, 116.42, 115.97, 95.55, 62.24, 39.90, 29.58, 26.77. MS (ESI) *m/z:* 606.8 $[M+H]^+$. Anal. Calcd for ($C_{35}H_{36}FN_50_2Si$): C, 69.39; H, 5.99; N, 11.56. Found: C, 69.38; H, 6.05; N, 11.50.

2-((2-(4-(4-Fluorophenylamino)-6-(2-hydroxyethyl)pyrimidin-2-yl)hydrazono)methyl) phenol (22).

2-((2-(4-(2-(tert-Butyldiphenylsilyloxy)ethyl)-6-(4-fluorophenylamino)pyrimidin-2-yl) hydrazono)methyl)phenol (0.025 mmol) was dissolved in dry THF (2 mL), triethylamine trihydro fluoride (24 μL, 0.150 mmol) was added and the resulting mixture was stirred overnight at r.t.. $NaHC0_3$ solution was added to the reaction mixture, then it was extracted with EtOAc, dried over Na_2S0_4 and evaporated. The crude material was dissolved in CH_2C1_2 and precipitated by petroleum ether to give the pure product **22** without further purification. Yield = 73%. ^1H NMR (400 MHz, CD30D-<¾): δ (ppm) 8.27 (s, 1H), 7.73 (m, 2H), 7.43 (m, 1H), 7.26 (t, *J* = 8 Hz, 1H), 7.1 (t, *J* = 8 Hz, 2H), 6.92 (q, *J* = 8 Hz, 2H), 6.17 (s, 1H), 3.94 (t, *J* = 6 Hz, 2H), 2.8 (t, *J* = 6 Hz, 2H). ^{13}C NMR (50 MHz, $CDCl_3$-*d*): δ (ppm) 163.22, 158.79, 145.46, 131.71, 130.35, 123.54, 123.49, 120.43, 117.32, 116.55, 116.10, 99.32, 61.44, 39.53, 30.77. MS (ESI) *m/z:* 368.4 $[M+H]^+$. Anal. Calcd for ($Ci_9Hi_8FN50_2$): C, 62.12; H, 4.94; N, 19.06. Found: C, 62.10; H, 4.98; N, 19.00.

EXAMPLE 6



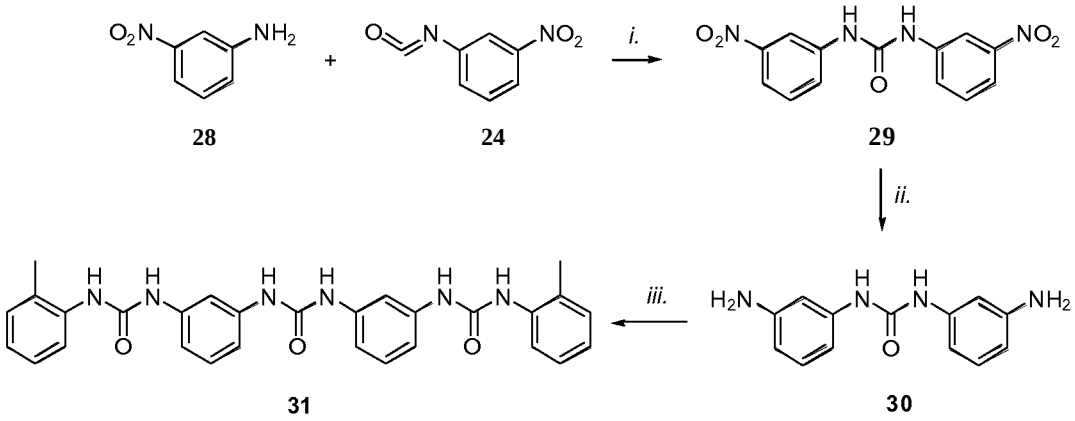
Reagents and conditions: *i.* CH_2Cl_2, r.t., 2 h; *ii.* Fe, HCl, EtOH/H_2O, reflux, 90 min; *iii.* KOCN, AcOH/H_2O.

l-(3-nitrophenyl)-3-o-tolylurea (25): 2-amino toluene **23** (300 mg, 300 µL, 2.80 mmol, 1 eq.) was added to a solution of 3-nitrophenyl isocyanate **24** (460 mg, 2.80 mmoL,l eq.) in anhydrous CH_2CI_2 (8 mL) in one portion. The solution was stirred for 2 hours at room temperature under a nitrogen atmosphere. The white precipitate was filtered, washed with petroleum ether and dried under high vacuum affording 750 mg (99%) of the desired product as a white solid. Further purification was unnecessary. H NMR (400 MHz, MeOD): δ: 2.31 (s, 3H, CH_3); 7.04-7.07 (t, J=8, 1H), 7.17-7.22 (m, 2H), 7.49-7.53 (t,J=8, 1H); 7.62-7.64 (d, J=8 1H); 7.73-7.75 (d, J=8, 1H); 7.85-7.87 (d, J=8, 1H); 8.50 (s, 1H;) Ms (ESI) *m/z:* 272 $[M+H]^+$ Anal. Calcd for ($Ci_4Hi_3N_30_3$): C, 61.99; H, 4.83; N, 15.49. Found: C, 62.00; H, 4.88; N, 15.40.

l-(3-aminophenyl)-3-o-tolylurea (26): Iron powder (423 mg, 7.56 mmol, 2 1 eq.), water (2 mL) and HC1 (2 drops) were added consecutively to a solution of **25** (100 mg, 0.36 mmol, 1 eq.) in ethanol (10 mL). After stirring at 95° for 90 min, the reaction mixture was filtered hot. Following an ethanol wash, the filtrates were combined and the solvent removed in vacuo. The crude material was purified by flash chromatography (60:40 ethyl acetate/petroleum ether) to provide **25** (70 mg, 0.29 mmol, 78%) as yellow solid

H NMR (400 MHz, MeOD): δ: 2.28 (s, 3H, CH_3); 6.45-6.48 (d, J=8, 1H); 6.69-6.71 (d, J=8, 1H); 6.91 (s, 1H), 7.00-7.03 (m, 2H), 7.15-7.17 (m, 2H), 7.61-7-63 (d, J=8, 1H) Ms (ESI) *m/z:* 242 $[M+H]^+$ Anal. Calcd for ($Ci_4Hi_5N_30$): C, 69.69; H, 6.27; N, 17.41. Found: C, 69.64; H, 6.29; N, 17.40.

l-[3-(carbamoylamino)phenyl]-3-(2-methylphenyl)urea (27): The urea derivative **26** (20 mg, 0.08 mmol,l eq.) was dissolved in acetic acid concentrated/water (1:1). To this a suspension of potassium cyanate (7 mg, 0.08 mmol,l eq.) in warm water was added. The reaction mixture was stirred for 30 min and then it was cooled in ice bath and filtered to obtain the desired product **27** (12 mg, 0.04 mmol, 52%) as white solid. Further purification was unnecessary. ¾ NMR (400 MHz, DMSO): : 2.15 (s, 3H, CHs); 5.74 (S, 2H, NH_2); 6.84 (m, 2H); 7.01-7.09 (m, 4H); 7.54 (s, 1H); 7.76-7.79 (m, 2H); 8.44 (s, 1H); 8.94 (s, 1H). Ms (ESI) *m/z:* 285 $[M+H]^+$Anal. Calcd for ($C_{15}H_{16}N_4O_2$): C, 63.37; H, 5.67; N, 19.71. Found: C, 63.38; H, 5.60; N, 19.77.



Reagents and conditions: *i.* CH_2CI_2, r.t., 2 h; *ii.* Fe, HC1, EtOH/H_20 , reflux, 90 min; *Hi.* o-tolyl isocyanate, dioxane dry, r.t.

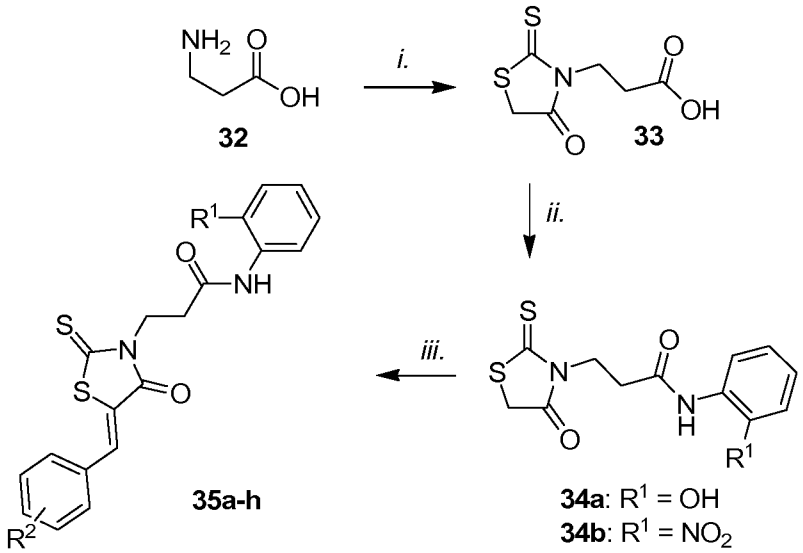
l,3-bis(3-nitrophenyl) urea (29): 3-nitroaniline **28** (300 mg, 2.18 mmol, 1 eq.) was added to a solution of 3-nitrophenyl isocyanate (357 mg, 2.18 mmol, 1 eq.) in anhydrous CH_2C1_2 (8 mL) in one portion. The solution was stirred for 2 hours at room temperature under a nitrogen atmosphere. The white precipitate was filtered, washed with petroleum ether Drying under high vacuum afforded 550 mg (83%) of the desired product **29** as a white solid. Further purification was unnecessary. H NMR (400 MHz, MeOD): δ: 7.51-7.55 (t, J= 8, 2H); 7.78-7.80 (d, J= 8, 2H); 7.88-7.90 (d, J= 8, 2H); 8.51 (s, 2H); Ms (ESI) *m/z:* 302 $[M+H]^+$Anal. Calcd for ($Ci_3HioN_40_5$): C, 51.66; H, 3.33; N, 18.54. Found: C, 51.69; H, 3.27; N, 18.60.

l,3-bis(3-aminophenyl)urea (30): Iron powder (190 mg, 3.36 mmol, 21 eq.), water (2 mL) and HC1 (2 drops) were added consecutively to a solution of **29** (50 mg, 0.16 mmol, 1 eq.) in ethanol (8 mL). After stirring at 95° for 90 min, the reaction mixture was filtered

hot. Following an ethanol wash, the filtrates were combined and the solvent removed in vacuo. The crude material was purified by flash chromatography (95:5 ethyl acetate/petroleum ether) to provide **30** (32 mg, 0.13 mmol, 80%) as yellow solid ^{1}H NMR (400 MHz, MeOD): δ: 6.37-6.41 (t, J= 8, 2H); 6.65-6.69 (t, J= 8, 2H); 6.86-6.88 (d, J= 8, 2H); 6.97-7.02 (q, J= 8, 2H); Ms (ESI) *m/z:* 243 $[M+H]^+$ Anal. Calcd for ($C_{13}H_{14}N_4O$): C, 64.45; H, 5.82; N, 23.13. Found: C, 64.44; H, 5.78; N, 23.18.

l,3-bis(3-{[(2-methylphenyl)carbamoyl]amino}phenyl)urea (31): A solution of o-tolyl-isocyanate (22 mg, 21 µL, 0.16 mmol, 1 eq.) in anhydrous dioxane (1 mL) was slowly added to a solution of **30** (20 mg, 0.08 mmol, 1 eq.) in anhydrous dioxane (1 mL). The reaction mixture was stirred for 24 h at room temperature. The solvent was removed under vacuum; the residual white solid was washed with ethanol, diethyl ether and hexane and filtered. Drying under high vacuum afforded 22 mg (52%) of the desired product **31** as a white solid. Further purification was unnecessary. ^{1}H NMR (400 MHz, MeOD): δ: 2.16 (s, 6H); 6.84-6.87 (t, J= 8, 2H); 6.93-6.95 (d, J= 8, 2H); 7.00-7.10 (m, 8H); 7.66 (s, 2H), 7.78 (s, 2H); 8.55 (s, 2H); 8.97 (s, 2H); Ms (ESI) *m/z:* 509 $[M+H]^+$ Anal. Calcd for ($C_{29}H_{28}N_6O_3$): C, 68.49; H, 5.55; N, 16.52. Found: C, 68.45; H, 5.50; N, 16.54.

EXAMPLE 7



Reagents and conditions: *i.* CS_2, $BrCH_2COOH$, 22% aq. KOH, r.t., 6 h; *ii.* pivaloyl chloride, DIPEA, 2-aminophenol, 1,2-dichloroethane, r.t., 18 h (for **34a);** $SOCl_2$, 2-

nitroaniline, CH_2Cl_2, r.t., 2 h (for **34b);** *Hi.* R^2PhCHO, EtOH, triethylamine, 1 h, reflux (Method A); R^2PhCHO, MW, 130 °C, 5 min (3 cycles) (Method B).

3-(4-Oxo-2-thioxothiazolidin-3-yl)propanoic acid (33). To a solution of β-alanine **32** (3.4 g, 38.1 mmol) in 17 mL of 22% KOH solution, CS_2 2.5 mL (42 mmol) was added dropwise making sure the temperature of the reaction did not exceed 25 °C. The mixture was allowed to stir at r.t. for approximately 3 hours and then bromoacetic acid (5.3 g, 38.1 mmol) was added portionwise over 20 minutes. The reaction mixture was stirred at room temperature for additional 3 hours during which time a precipitate was formed. The pH of the reaction mixture was adjusted to 3-4 using cone. H_2SO_4 and the resulting solution was stirred overnight at room temperature. The precipitate was filtered off and washed with water thus obtaining the desired pure compound **33** (3.52 g, yield 45%) as a yellow solid. Mp 155-156 °C. ^1H NMR (400 MHz, MeOD-d_4) δ (ppm) 5.00 (brs, 1H), 4.22 (t, J = 7.5, 2H), 4.11 (s, 1H), 2.64 (t, J = 7.6, 2H). ^{13}C NMR (100 MHz, MeOD-d_4) δ (ppm) 202.58, 174.37, 172.87, 39.64, 35.08, 30.28. MS (ESI) *m/z*: 204.1 [M-H]\ Anal. Calcd for ($C_6H_7NO_3S_2$): C, 35.11; H, 3.44; N, 6.82. Found: C, 35.10; H, 3.48; N, 6.88.

7V-(2-Hydroxyphenyl)-3-(4-oxo-2-thioxothiazolidin-3-yl)propanamide (34a). Compound **33** (1.0 g, 4.87 mmol) and *N*,*N*-diisopropylethylamine (932 μL, 5.36 mmol) were dissolved in 20 mL of dry 1,2-dichloroethane and finally pivaloyl chloride (660 μL, 5.36 mmol) was added dropwise. The reaction mixture was stirred at room temperature for 3 hours and then 2-aminophenol (531 mg, 4.87 mmol) was added. The mixture was allowed to stir at room temperature for additional 18 hours. The solvent was removed under reduced pressure and the mixture was purified with flash chromatography (hexane/EtOAc:l/l) to give the desired product **34a** (1.233 g, yield 85%) as a yellow solid. Mp 168-170 °C. ^1H NMR (400 MHz, DMSO-d_6) δ (ppm) 9.65 (s, 1H), 9.36 (s, 1H), 7.63 (d, J = 7.7 1H), 6.95-6.91 (m, 1H) 6.83 (d, J = 7.8, 1H) 6.75-6.72 (m, 1H), 4.24 (s, 2H), 4.13 (t, J = 7.4, 2H), 2.68 (t, J = 7.5, 2H). ^{13}C NMR (50 MHz, DMSO-d_6) δ (ppm) 202.75, 173.98, 168.50, 148.10, 125.77, 124.74, 122.85, 118.75, 115.62, 38.2, 35.71, 32.57. MS (ESI) *mlz*: 295.4 $[M-H]^-$. Anal. Calcd for ($Ci_2HiiN_2O_3S_2$): C, 48.63; H, 4.08; N, 9.45. Found: C, 48.66; H, 4.04; N, 9.40.

7V-(2-Nitrophenyl)-3-(4-oxo-2-thioxothiazolidin-3-yl)propanamide (34b). To a suspension of **33** (100 mg, 0.48 mmol) in 4 mL of dry dichloromethane, thionyl chloride (40 μL, 0.58 mmol) was added. The reaction was monitored by TLC and after the

disappearance of the starting material, 2-nitroaniline (80 mg, 0.58 mmol) was added. The resulting mixture was stirred at room temperature for 2 hours. H_20 was added to the reaction mixture, then it was extracted with EtOAC, dried over Na_2S0_4, concentrated under reduced pressure and purified with flash chromatography (hexane/EtOAc:l/l) to give the desired product **34b** (130 mg, yield 84%) as a yellow solid.

Mp 170-171 °C. ¹H NMR (400 MHz, *CDCl₃-d)* δ (ppm) 10.27 (s, 1H), 8.64-8.62 (m, 1 H), 8.15-8.13 (m, 1H), 7.60-7.56 (m, 1H), 7.15-7.1 1 (m, 1H), 4.45 (t, *J* = 8, 2H), 3.94 (s, 2H), 2.22 (t, *J* = 8, 2H). ^{13}C NMR (100 MHz, *OMSO-d_6)* δ (ppm) 206.19, 173.99, 168.83, 136.04, 134.16, 128.02, 125.78, 123.59, 122.38, 40.28, 35.43, 34.87. MS (ESI) *m/z:* 324.4 [M-H]⁻. Anal. Calcd for ($Ci_2HiiN_30_4S_2$): C, 44.30; H, 3.41; N, 12.91. Found: C, 44.36; H, 3.38; N, 12.90.

General procedure for the synthesis of 35a-h (Method A).

To a solution of the opportune intermediate **34a** or **34b** (0.33 mmol) in 4 mL of EtOH, the opportune benzaldehyde (0.33 mmol) and triethylamine (0.33 mmol) were added. The reaction mixture was refluxed for 1 hour then the precipitate formed was filtered off and washed with EtOH and hexane to give the pure products.

General procedure for microwave-assisted synthesis of 35a-h (Method B). A mixture of the opportune intermediate **34a** or **34b** (0.16 mmol) and the appropriate benzaldehyde (0.16 mmol) was irradiated in the microwave for 5 min at 130 °C (3 cycles). The residue was washed with EtOH and hexane to give the desired pure compounds.

(Z)-3-(5-(3-Bromobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-7V-(2-hydroxy phenyl)propanamide (35a; FE15). Yellow solid. Mp 222-224 °C. ¹H NMR (400 MHz, DMSO-*d₆*) δ (ppm) 9.56 (s, 1H), 9.38 (s, 1H), 7.89 (s, 1 H), 7.81 (s, 1H), 7.71 (d, *J* = 7.9 1H), 7.65-7.60 (m, 2H), 7.53-7.49 (m, 1H), 6.92-6.90 (m, 1H) 6.83 (d, *J* = 7.8, 1H) 6.75-6.72 (m, 1H), 4.32 (t, *J* = 7.1, 2H), 2.79 (t, *J* = 7.1, 2H). ^{13}C NMR (100 MHz, DMSO-*d₆*) δ (ppm) 193.37, 169.07, 167.08, 148.66, 135.86, 133.87, 133.85, 132.00, 131.45, 129.04, 126.38, 125.30, 124.72, 123.36, 123.07, 119.33, 116.13, 41.40, 33.39. MS (ESI): *m/z* 462.9 [M-H]⁺; Anal. Calcd for ($Ci_9Hi_5BrN_20_3S_2$): C, 49.25; H, 3.26; N, 6.05. Found: C, 49.31; H, 3.29; N, 6.06.

3-((Z)-5-(3-Fluorobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-hydroxyphenyl) propanamide (35b). Yield 45%. Yellow solid. Mp 210-21 1 °C. ¹H NMR (400 MHz, acetone-^): δ (ppm) 9.17 (s, 1H), 7.69 (s, 1H), 7.59-7.54 (m, 1H), 7.44-7.41 (m, 1H), 7.37 (d, *J* = 8, 1H), 7.26-7.21 (m, 1H), 6.97-6.92 (m, 1H), 6.82 (d, *J* = 8 1H), 6.76-6.72 (m,

1H), 4.45 (t, *J* = 7.1, 2H), 2.92 (t, *J* = 7.1, 2H). ^{13}C NMR (75 MHz, DMSO-<¾): δ (ppm) 193.68, 169.30, 167.37, 164.65, 161.39, 148.88, 136.05, 135.94, 132.35, 132.23, 131.96, 126.77, 126.73, 126.60, 126.52, 124.86, 123.59, 119.55, 118.53, 118.24, 118.17, 117.88, 116.34, 40.94, 33.29. MS (ESI) *mlz:* 401.5 [M-H]$^-$. Anal. Calcd for **(C19H15FN2O3S2):** C, 56.70; H, 3.76; N, 6.96. Found: C, 56.76; H, 3.75; N, 6.98.

3-((Z)-5-(3,5-Difluorobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-hydroxyphenyl) propanamide (35c). Yield 77%. Yellow solid. Mp 235-237 °C. ^{1}H NMR (400 MHz, DMSO-<¾): δ (ppm) 9.56 (s, 1H), 9.30 (s, 1H), 7.72 (s, 1H), 7.58-7.56 (m, 1H), 7.37-7.33 (m, 1H), 7.28-7.27 (m, 2H), 6.87-6.83 (m, 1H), 6.77-6.75 (m, 1H), 6.68-6.64 (m, 1H), 4.23 (t, *J* = 7.16, 2H), 2.70 (t, *J* = 7.16, 2H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ (ppm) 193.05, 168.97, 166.96, 164.36, 164.22, 161.89, 161.76, 148.57, 136.72, 130.27, 126.30, 126.11, 125.21, 123.26, 119.25, 116.04, 113.71, 113.44, 106.77, 106.51, 106.25, 41.35, 33.28. MS (ESI) *mlz:* 419.4 [M-H]$^-$. Anal. Calcd for ($C_{19}H_{14}F_2N_2O_3S_2$): C, 54.28; H, 3.36; N, 6.66. Found: C, 54.30; H, 3.30; N, 6.68.

3-((Z)-5-(3-Methylbenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-hydroxyphenyl) propanamide (35d). Yield 61%. Yellow solid. Mp 208-209 °C. ^{1}H NMR (400 MHz, DMSO-<¾): δ (ppm) 9.57 (s, 1H), 9.30 (s, 1H), 7.69 (s, 1H), 7.57 (d, *J* = 8, 1H), 7.39-7.36 (m, 3H), 7.27-7.25 (m, 1H), 6.87-6.83 (m, 1H), 6.76 (d, *J* = 8, 1H), 6.69-6.64 (m, 1H), 4.25 (t, *J* = 7.2, 2H), 2.72 (t, *J* = 7.2, 2H). ^{13}C NMR (100 MHz, DMSO-<¾): δ (ppm) 193.67, 169.01, 167.15, 148.56, 139.31, 133.36, 132.12, 131.43, 129.81, 128.21, 126.32, 125.21, 123.26, 122.64, 119.26, 116.07, 41.22, 33.32, 21.28. MS (ESI) *mlz:* 397.5 [M-H]$^-$. Anal. Calcd for **(C20H18N2O3S2):** C, 60.28; H, 4.55; N, 7.03. Found: C, 60.21; H, 4.59; N, 7.12.

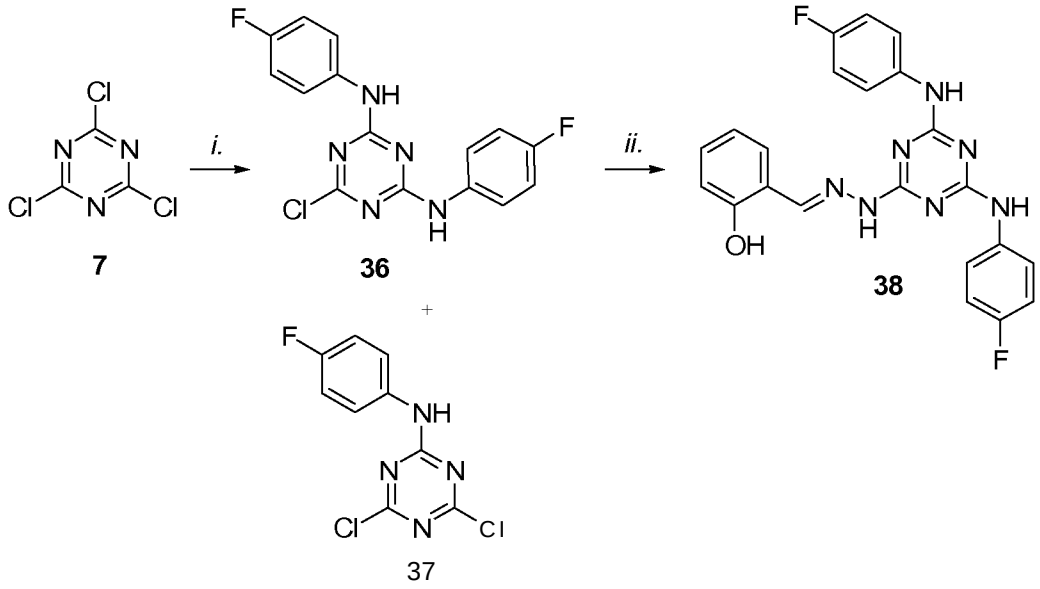
3-((Z)-5-(3-Methoxybenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-hydroxyphenyl) propanamide (35e). Yield 67%. Yellow solid. Mp 200-202 °C. ^{1}H NMR (400 MHz, DMSO-<¾): δ (ppm) 9.31 (s, 1H), 7.73 (s, 1H), 7.57 (d, *J* = 8, 1H), 7.42-7.38 (m, 1H), 7.14-7.12 (m, 2H), 7.03-7.01 (m, 1H), 6.87-6.83 (m, 1H), 6.76 (d, *J* = 8, 1H), 6.68-6.64 (m, 1H), 4.25 (t, *J* = 7.2, 2H), 2.72 (t, *J* = 7.2, 2H). ^{13}C NMR (100 MHz, DMSO-<¾): δ (ppm) 193.68, 169.10, 160.23, 148.68, 134.84, 133.29, 131.13, 126.40, 125.30, 123.37, 122.94, 119.33, 117.47, 116.26, 116.15, 55.83, 41.35, 33.41. MS (ESI) *mlz:* 413.5 [M-H]$^-$. Anal. Calcd for **(C20H18N2O4S2):** C, 57.95; H, 4.38; N, 6.76. Found: C, 57.97; H, 4.44; N, 6.70.

3-((Z)-5-((Benzo[i/][l,3]dioxol-5-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-hydroxy phenyl)propanamide (35f). Yield 53%. Yellow solid. Mp 240-241 °C. ¹H NMR (400 MHz, DMSO-<¾): δ (ppm) 9.56 (s, 1H), 9.30 (s, 1H), 7.66 (s, 1H), 7.58-7.56 (m, 1H), 7.14-7-12 (m, 1H), 7.09 (s, 1H), 7.04-7.01 (m, 1H), 6.87-6.84 (m, 1H), 6.77-6.75 (m, 1H), 6.68-6.65 (m, 1H), 6.07 (s, 2H), 4.23 (t, *J* = 7.2, 2H), 2.70 (t, *J* = 7.2, 2H). ^{13}C NMR (100 MHz, *OMSO-d_6):* δ (ppm) 193.29, 169.03, 167.18, 150.29, 148.77, 148.57, 133.53, 127.61, 127.40, 126.32, 125.20, 123.26, 120.18, 119.26, 116.07, 110.01, 109.74, 102.60, 41.19, 33.32. MS (ESI) *m/z:* 427.0 [M-H]⁻. Anal. Calcd for ($C_{20}Hi_6N_20_5S2$): C, 56.06; H, 3.76; N, 6.54. Found: C, 56.03; H, 3.84; N, 6.51.

3-((Z)-5-(3-Bromobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-nitrophenyl)propanamide (35g). Yield 85%. Yellow solid. Mp 204-206 °C. ¹H NMR (400 MHz, DMSO-<¾): δ (ppm) 10.32 (s, 1H), 7.87-7.84 (m, 1H), 7.79 (s, 1H), 7.72 (s, 1H), 7.63-7.60 (m, 2H), 7.54-7.52 (m, 2H), 7.45-7.41 (m, 1H), 7.31-7.27 (m, 1H), 4.23 (t, *J* = 7.4, 2H), 2.70 (t, *J* = 7.4, 2H). ^{13}C NMR (100 MHz, DMSO-<¾): δ (ppm) 193.43, 168.87, 166.99, 142.99, 135.76, 134.32, 133.78, 131.93, 131.39, 131.18, 128.95, 126.00, 125.84, 125.24, 124.66, 123.00, 40.86, 33.20. MS (ESI) *m/z:* 491.4 [M-H]⁻. Anal. Calcd for ($Ci_9Hi_4BrN30_4S_2$): C, 46.35; H, 2.87; N, 8.53. Found: C, 46.42; H, 2.85; N, 8.56.

3-((Z)-5-(3-Fluorobenzylidene)-4-oxo-2-thioxothiazolidin-3-yl)-N-(2-nitrophenyl)propanamide (35h). Yield 77%. Yellow solid. Mp 207-208 °C. ¹H NMR (400 MHz, DMSO-<¾): δ (ppm) 10.32 (s, 1H), 7.87-7.85 (m, 1H), 7.74 (s, 1H), 7.64-7.60 (m, 1H), 7.54-7.52 (m, 2H), 7.45-7.42 (m, 1H), 7.39-7.37 (m, 1H), 7.31-7.27 (m, 2H), 4.23 (t, *J* = 8, 2H), 2.70 (t, *J* = 8, 2H). ^{13}C NMR (100 MHz, DMSO-<¾): δ (ppm) 193.61, 168.95, 167.14, 164.03, 161.58, 143.09, 135.81, 135.73, 134.39, 132.11, 132.03, 131.75, 131.26, 126.52, 126.08, 125.92, 125.32, 124.68, 118.27, 118.06, 117.90, 117.67, 40.94, 33.29. MS (ESI) *m/z:* 430.5 [M-H]⁻. Anal. Calcd for ($Ci_9Hi_4FN_30_4S_2$): C, 52.89; H, 3.27; N, 9.74. Found: C, 52.80; H, 3.26; N, 9.81.

EXAMPLE 8



Reagents and conditions: *i.* DME, -30 °C, 4-fiuoroaniline, 3 h; *ii.* a) CH_2Cl_2, NH_2NH_2 H_20, reflux, 12 h; b) toluene, salicylaldehyde, 3 h, reflux, Dean-Stark.

6-Chloro-7V2,/V4-bis(4-fluorophenyl)-l,3,5-triazine-2,4-diamine (36): To a stirred solution of cyanuric chloride **7** (2g, 10.86 mmol) in dimethoxyethane (20 mL) at -30 °C, 4-fluoroaniline (1 eq) was added dropwise. The reaction mixture was vigorously stirred for 3 h at -30 °C then warmed up to r.t. and washed with 3N HCl, water, brine and finally dried over anhydrous Na_2S0_4. The organic phase was evaporated to dryness and the white residue was purified by flash chromatography (petroleum ether/Et_20 3/1) to give the desired product **36** and the side product **37.** Yield 50 %. ^{1}H NMR (400 MHz, *CDCl$_3$-d)*: δ (ppm) 7.79 (brs, 2H), 7.39-7.36 (m, 4H), 7.04-7.02 (m, 4H). MS (ESI) *m/z*: 30: 334.7 $[M+H]^+$;]$^+$. Anal. Calcd for ($Ci_5Hi_0ClF_2N_5$): C, 53.99; H, 3.02; N, 20.99. Found: C, 53.94; H, 3.05; N, 20.95.

4,6-Dichloro-/V-(4-fluorophenyl)-l,3,5-triazin-2-amine (37). Yield 35%;. Mp 172 °C;. ^{1}H NMR (400 MHz, *CDCl$_3$-d):* δ (ppm) 7.79 (brs, 1H), 7.41 (q, *J* = 8.60, 2H), 7.03 (t, *J* = 8.63, 2H). ^{13}C NMR (100 MHz, $CDCl_3$-*d*): δ (ppm) 171.28, 164.33, 161.68, 159.23, 131.62, 123.80, 116.26. MS (ESI) *m/z:* 260.1 $[M+H]^+$; 282.1 $[M+Na]^+$. Anal. Calcd for ($C_9H_5Cl_2FN_4$): C, 41.73; H, 1.95; N, 21.63. Found: C, 41.77; H, 1.93; N, 21.64.

(£)-2-((2-(4,6-bis(4-Fluorophenylamino)-l,3,5-triazin-2-yl)hydrazono)methyl)phenol (38): To a solution of **36** (1 eq) in dichloromethane, hydrazine (4 eq) was added and the resulting mixture was refluxed for 12 h. After cooling down to r.t., the mixture was washed with water, brine and finally dried over anhydrous Na_2S0_4. The organic phase was

evaporated to dryness, the residue was dissolved in toluene and reacted with salicylaldehyde (2 eq). The reaction mixture was refluxed for 3 h using a Dean-Stark apparatus for azeotropical removal of water and then evaporated to dryness. The resulting residue was dissolved in the minimum amount of dichloromethane; by addition of petroleum ether the desired final compounds were collected by filtration.

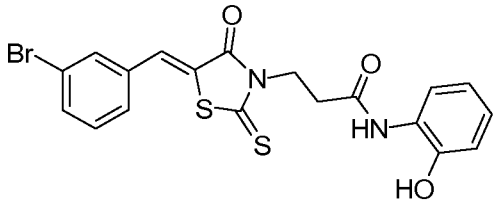
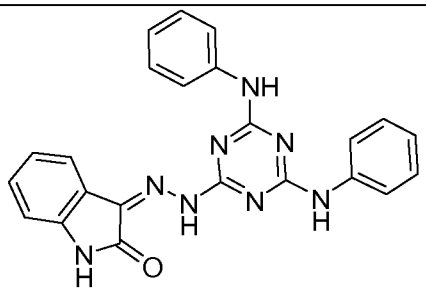
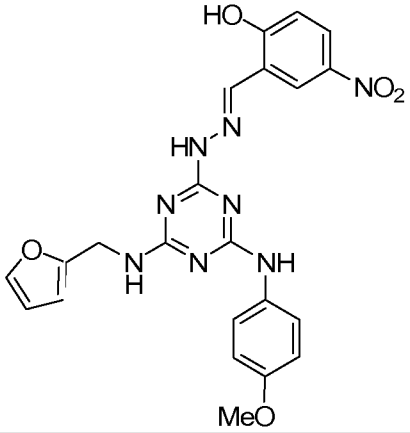
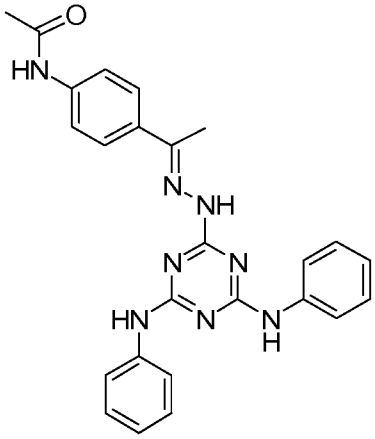
Yield 48%. ^{1}H NMR (400 MHz, *CDCl$_3$-d)*: δ (ppm) 11.20 (brs, 1H), 7.80 (s, 1H), 7.40 (brs, 3H), 7.22-7.19 (m, 2H), 7.04-7.02 (m, 1H), 6.96-6.94 (m, 4H), 6.82-6.78 (m, 1H). MS (ESI) *m/z:* 434.4 $[M+H]^+$. Anal. Calcd for ($C_{22}H_{17}F_2N_7O$): C, 60.97; H, 3.95; N, 22.62. Found: C, 60.94; H, 3.96; N, 22.55.

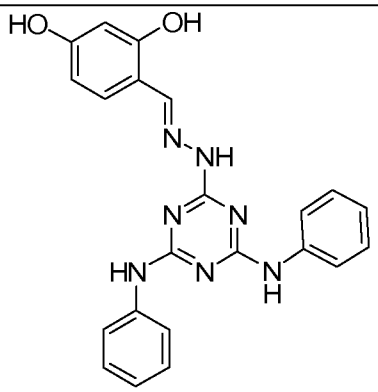
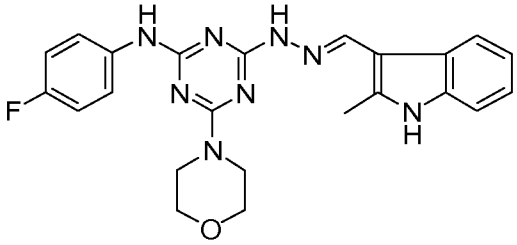
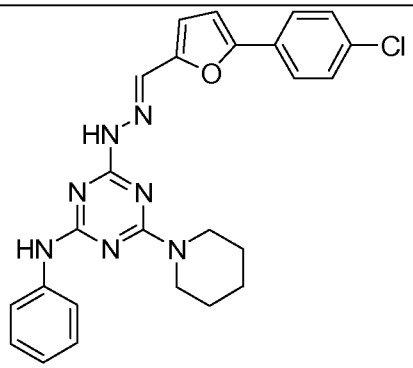
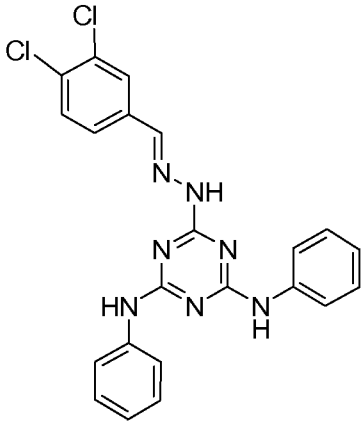
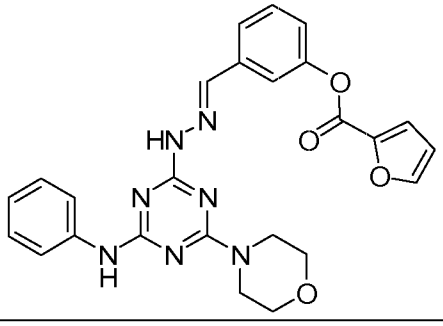
EXAMPLE 9

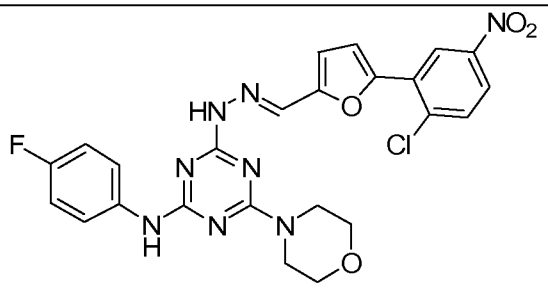
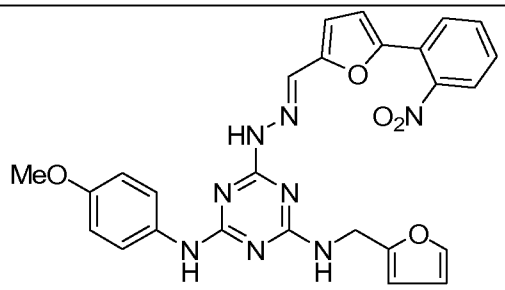
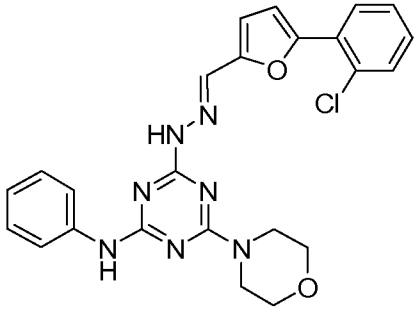
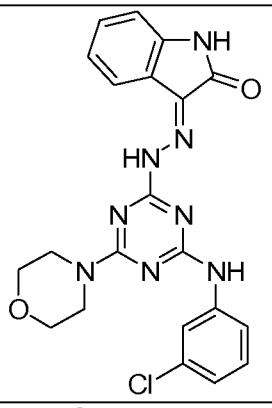
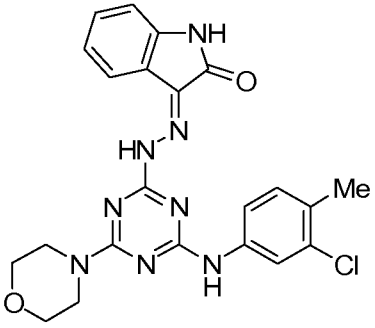
Anti-enzymatic activity:

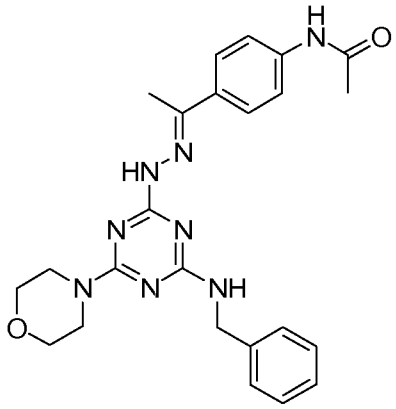
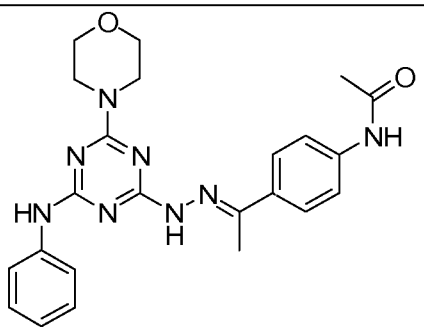
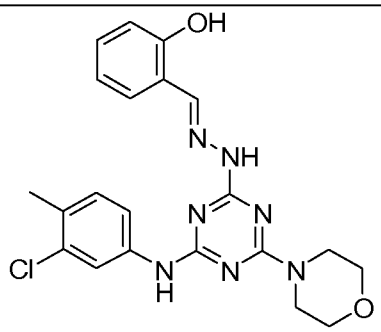
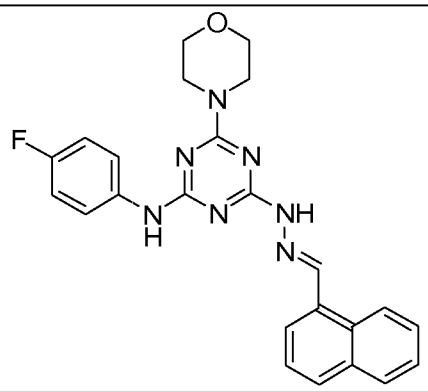
The anti-enzymatic activity of representative compounds of the invention against the DDX3 ATPase activity is reported in Table 1.

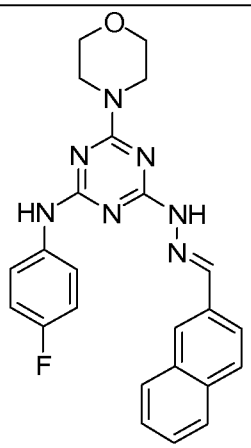
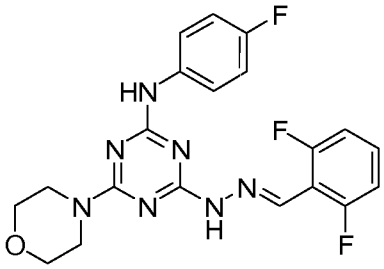
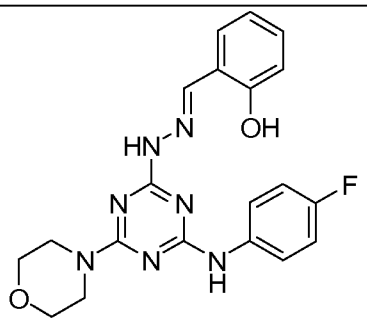
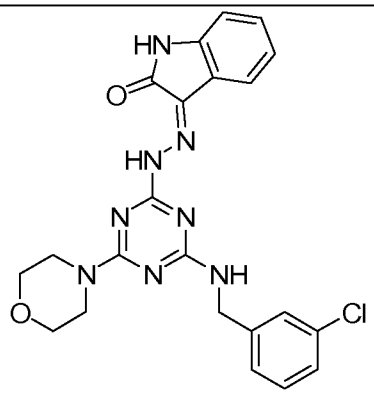
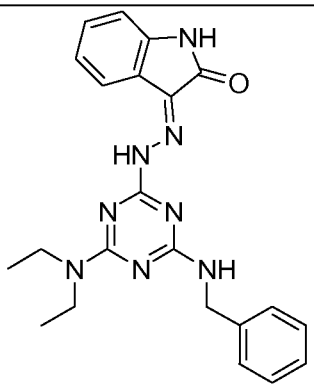
Table 1. Activity of representative compounds of the invention against DDX3 ATPase

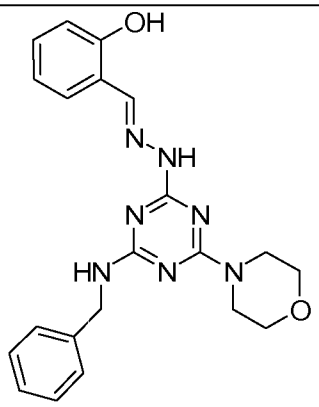
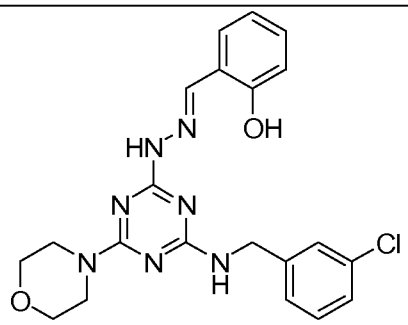
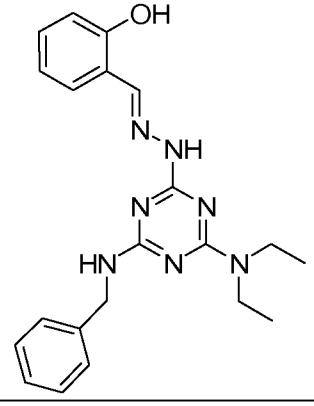
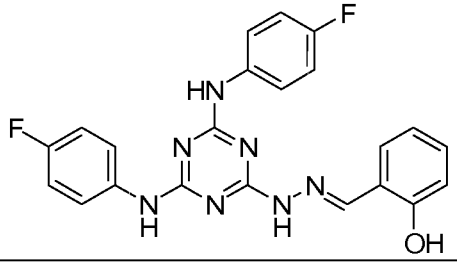
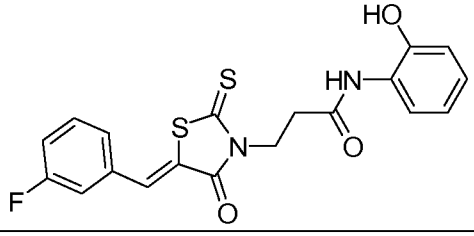
Compound ID [a]	Structure	Ki (μM) [b]
FE-15 (**35a**)		4.5
FE-56		0.4
FE-56A		31.7
FE-56F		0.3

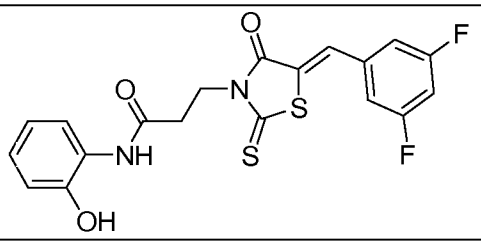
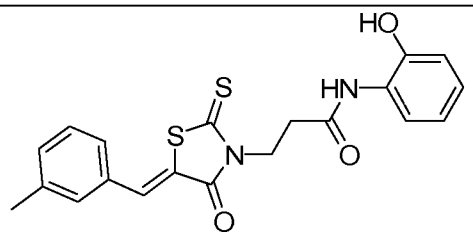
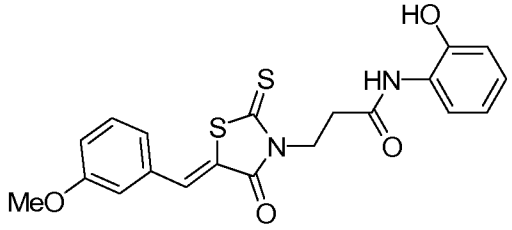
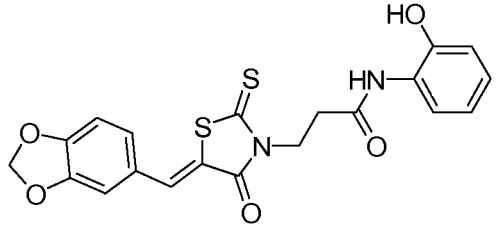
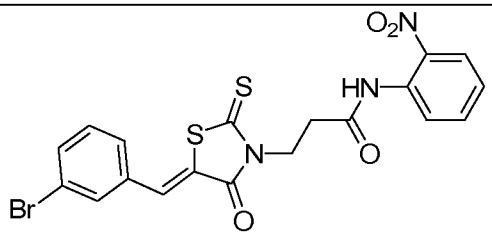
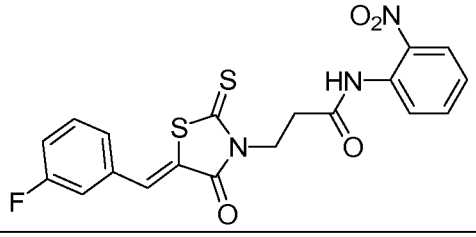
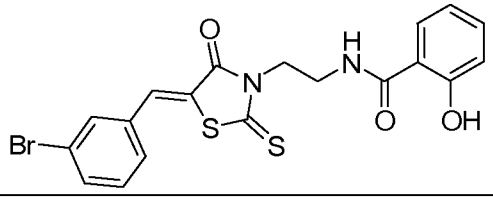
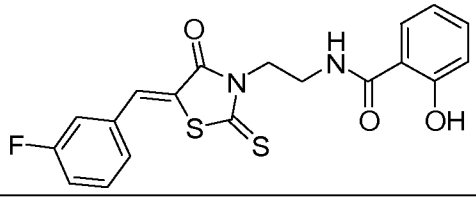
FE-56I		33
FE-56M		0.2
FE-56N		0.4
FE-56O		18
FE-56U		6.3

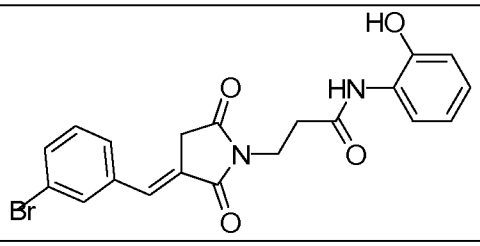
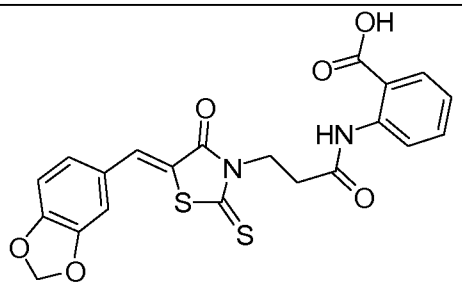
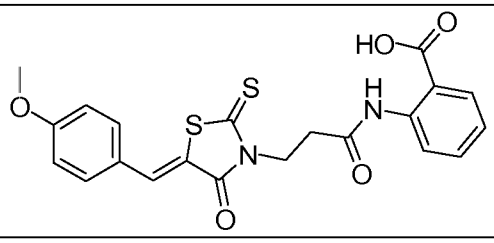
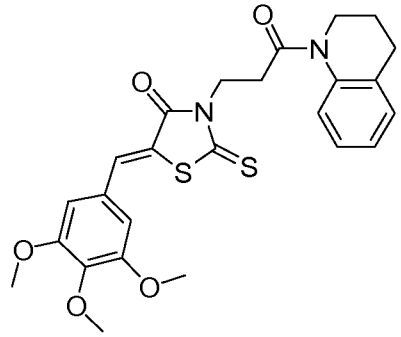
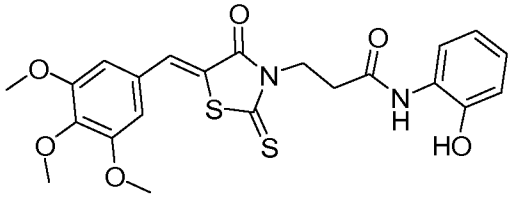
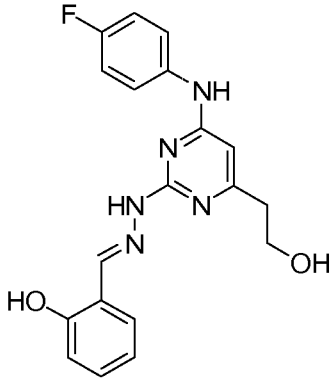
FE-56V		3.6
FE-56Z		1.9
FE-56AA		3.2
FE-56AD		2
FE-56AH		3.2

FE-56AN		0.5
FE-56AI		2.2
FE-56AM		1.6
11a		86

11b		8.5
11c		2.6
11d		0.4
14f		2.9
14g		0.1

15h		0.6
15j		62
15k		0.5
38		0.1
35b		0.3

35c		0.5
35d		97
35e		10
35f		1.0
35g		8.7
35h		7.6
3j		4.2
3k		4.3

6b		28
FE-70		0.4
FE-77		2.0
FE-69		0.9
FE-74		0.1
22		9.0

[a] FE-compounds were obatained by commercial sources (Asinex and ChemBridge) while the other were synthesized using the procedures reported in the examples 1-5 and 7-8. [b] Apparent equilibrium dissociation constant for the inhibitor to the target enzyme DDX3, expressed in micromolar concentration.

EXAMPLE 10

Antiviral activity:

Selected compounds from Table 1 were tested against HIV-1 replication in two different model systems. Figure 1 A shows the effects of compounds FE56 and **35b** against HIV-1 single-round replication in HeLaCD4+ cells infected with a wild type HIV-1 strain. The data clearly show a dose-dependent reduction of viral load (quantified as viral RNA copies), indicative of an inhibition of viral replication. Figure 1 B shows the effects of compounds FE15 and **35b** against multiple rounds of replication of wild type HIV-1 in natural target cells (PBMC). The data clearly show a significant reduction of viral RNA at 5 days post infection. Together, the data presented in Figure 1 clearly demonstrate that selected compounds of the invention are capable to inhibit HIV-1 replication in two different model systems.

It is interesting to note that the inhibitor **FE15** displayed very low cytotoxicity on HeLa cells (CC_{so} > 200 μM) but only modest anti-HIV activity (EC_{50} = 83 μM).

Figure 2A shows the antiviral activity of **FE15** on PBMCs infected with HIV-1, in comparison with the most potent derivatives **35b, lid** and **38.** It can be appreciated that the compounds **lid** and **38** showed between 40% and 60% reduction of viral load already at 3 μM, while **FE15** needed to be added at 50 μM to show comparable effects. Dose response curves were generated for **FE15** and **38.** As shown in Figure 2B, **38** showed a 41- fold higher antiviral potency on HIV-1 infected PBMCs (EC_{50} = 2 μM) than the inhibitor **FE15** (EC_{50} = 83 μM). Similar curves yielded EC_{50} values for **35b** and **lid** of 7.5 and 2.5 μM, respectively. The antiviral potencies and toxicity indexes of the most active compounds are summarized in the Table 2 below.

Table 2. Antiviral and cytotoxic activity of selected compounds

Comd.	Antiviral activity[a]	Cytotoxicity (CC50)[b]			Selectivity index[c]		
		HeLa	MOLT-4	PBMCS	HeLa	MOLT-4	PBMCs
FE15 (35a)	83±7	>200	>200	>150	2.4	2.4	1.8
FE66 (35b)	7.5±0.7	50±5	50±10	50±5	6.7	6.7	6.7
16c	2.5±0.1	2.5±0.3	5±1	lOthl	**1.0**	2.0	4.0
38	2.0±0.2	20±2	l O±l	8.0±0.5	10	5.0	4.0

a. dose required to reduce 50% viral proliferation (measured as viral RNA load)
b. dose requried to reduce 50% cell vitality
c. Expressed as CC50/EC50

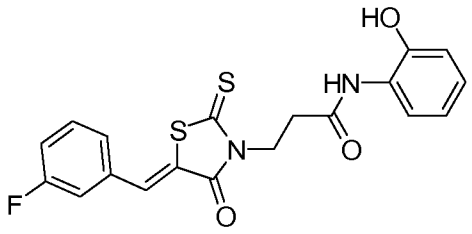
The data shown in Table 2, clearly demonstrate the ability of the compounds of the invention to potently suppress cellular proliferation of the highly proliferating HeLa cancer cell line.

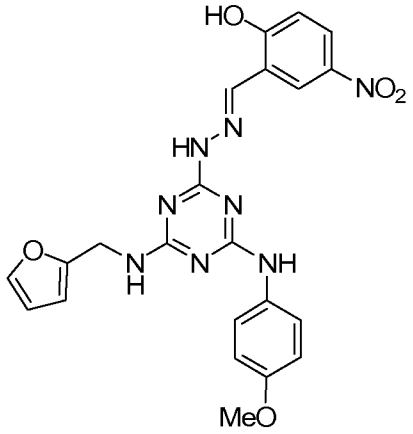
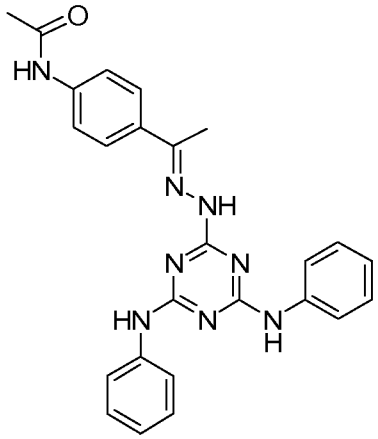
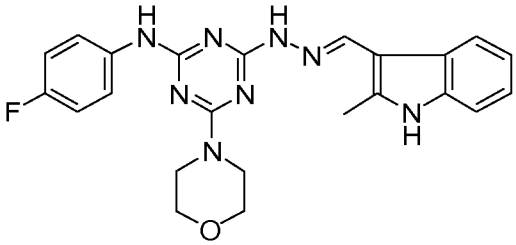
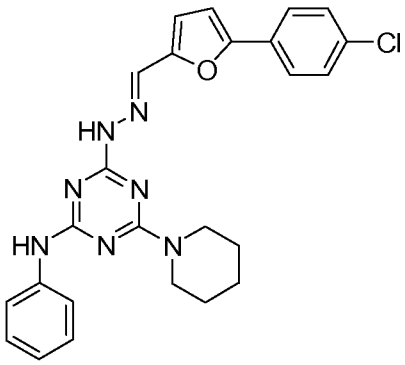
EXAMPLE 11

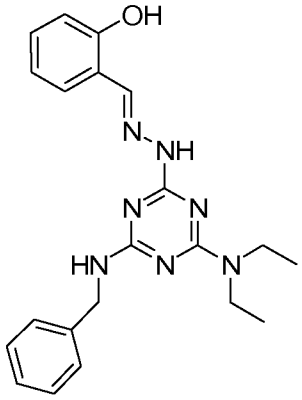
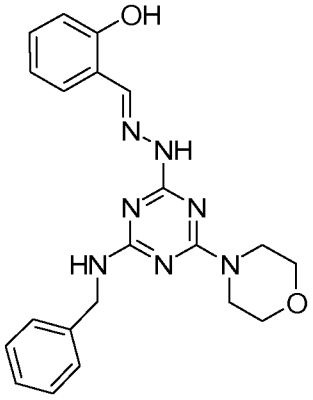
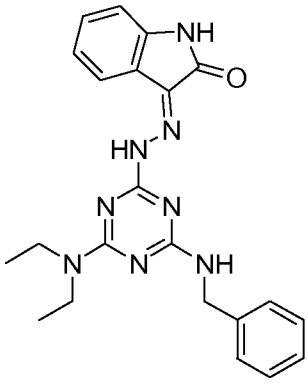
Antiproliferative activity:

Selected compounds from Table 1 were tested against the cervical cancer HeLa cell line for antiproliferative activity. Cell viability was measured with the CellTiter viability assay (Table 2). Table 3 lists the calculated antiproliferative potencies (EC_{50}, dose required to suppress 50% of cell viability) for a series of representative compounds of the invention.

Table 3. EC50 values for antiproliferative activity against HeLa cells

Compound ID [a]	Structure	EC50 (μM) 48 hours	EC50 (μM) 72 hours
35b		**50**	**10**

FE-56A		**8**	**4**
FE-56F		**10**	**5**
FE-56M		**10**	**5**
FE-56N		**25**	**4**

15k		**3**	**1**
15h		**5**	**2**
14g		**10**	**10**

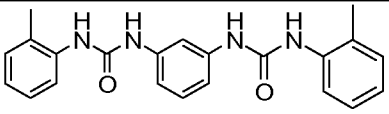
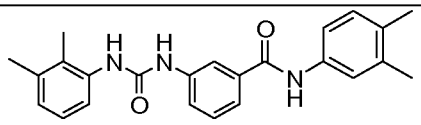
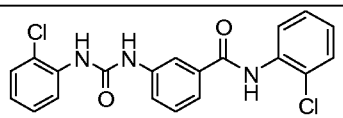
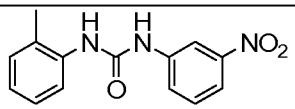
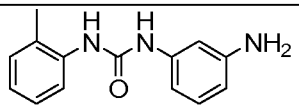
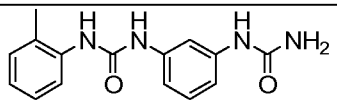
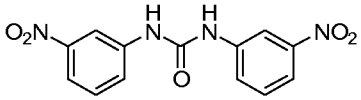
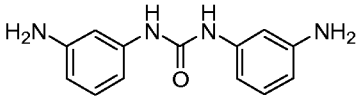
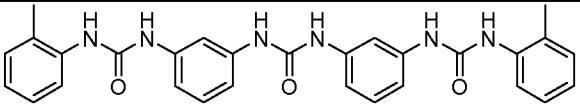
[a] FE-compounds were obatained by commercial sources (Asinex and ChemBridge) while the other were synthesized using the procedures reported in the examples 4 and 7.

Example 12. Anti-helicase activity

Compounds were obtained by application of a virtual docking protocol on the RNA-binding site identified in the homology model developed in the present invention. These compounds were commercially available **(El**-compounds in **Table 4).** A few other

compounds (25-31, EXAMPLE 6) were rationally designed to target the above mentioned RNA-binding site and then synthesized. All the compounds were tested for anti-helicase activity. The results are reported in Table 4.

Table 4: anti-helicase and ATPase activity of the compound of the invention

Compound ID[a]	**Structure**	**Helicase** ID50 (μM)	**ATPase** ID50 (μM)
EI-01		250	245
EI-01A		131	
EI-01B		1300	
25		1	11
26		5.7	
27		na [b]	
29		52	
30		24	
31		1300	

[a] El-compounds were obtained by commercial sources (Asinex and ChemBridge) while the other were synthesized using the procedures reported in the example 6. [b] na = not active

Among those of the first series, compound EI-01 proved to be the most potent, but did not discriminate between ATPase and helicase activities. Compounds 25 and 26 showed 245- and 43- fold improvement in their anti-helicase activity, with respect to EI01. Moreover,

compound **25** showed an 11-fold higher potency against the helicase, with respect to the ATPase activity.

RESULTS

The anti-DDX3 activity of the compounds of the invention was evaluated by in vitro ATPase activity assay using the recombinant human DDX3 protein produced in E.coli. The potency of inhibition (Ki) for each molecule was calculated, representing the concentration of the inhibitor able to reduce the DDX3 ATPase activity by 50%

The most active compounds were further optimized and tested in anti-HIV and antiproliferative cellular assays.

The results obtained and reported in the Examples show that the compounds of the invention were able to:

1) inhibit the ATPase activity of the human DDX3 protein by interacting with the ATP binding site and interfering with the subsequent catalytic steps through a mixed-type inhibitory mechanism;

2) suppress HIV-1 replication in infected cells with low toxicity to uninfected control cells;

3) suppress proliferation of the HeLa cervical cancer tumor cell line.

The data of the present invention demonstrate the capacity of the present compounds to inhibit proliferation of HIV-1 as well as cancer cells. For these reasons, such molecules, used alone or in synergy (cocktail), are suitable for the treatment of viral (e.g. HIV-1 and HCV) infections and for the treatment of diseases caused by uncontrolled cellular proliferation (cancer).

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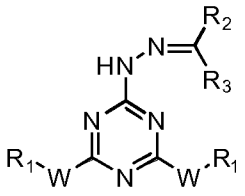
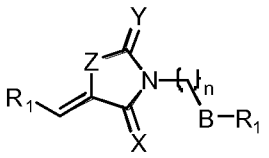
CLAIMS:

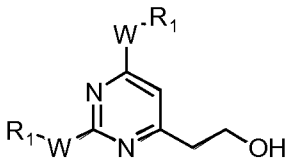
1- A compound of formula 1, 2, 3 or 4 for use as a treatment of a pathology modulated by DDX3 activity and/or expression:



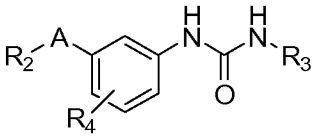
Formula 1



Formula 2



Formula 3



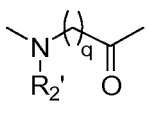
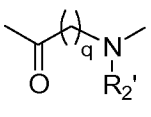
Formula 4

wherein:

Z represents CH_2 or S;

X and Y represent independently O or S;

n is comprised between 0 and 4;

B is absent or represents  ,  q is comprised between 0 and 2 and R_2' represents H, -$(CH_2)_W$'-OH, -(CH_2)w'-NH_2, w' is an integer from 1 to 3; B is also C=0;

Ri, R_2, R_3 are each independently selected from the group of: H, a linear or branched alkyl group comprising 1 to 6 carbon atoms, unsubstituted or substituted phenyl radical, an unsubstituted or substituted phenylalkenyl radical, an unsubstituted or substituted phenyalkynyl radical, an unsubstituted or substituted biphenylalkyl radical, an unsubstituted or substituted heterocyclic radical, an unsubstituted or substituted polycyclic radical, an unsubstituted or substituted alicyclic radical or a radical of the formula (Ria-)$_m$(L-)$_p$Rib-, wherein Ria and Rib may be the same or different and represent an unsubstituted or substituted heterocyclic radical or an unsubstituted or substituted phenyl radical, Ria also represents an unsubstitutetd or substituted polycyclic radical and L represents a divalent linking moiety selected from the group consisting of a valence bond, -

$(CH_2)q$-, -HC=CH-, -C≡C-, -C(=0)-, -0-, -S-, -S(=0)-, $-S(=0)_2$-, -NHCONH- or **NRjC, RiC** being hydrogen or alkyl, m and p are each independently 0 or 1, and q is an integer from 1 to 3;

$\mathbf{R_2}$ and $\mathbf{R_3}$ together optionally form a cycloalkyl, cycloalkenyl, non-aromatic heterocyclic, or fused or polycyclic ring, 2-oxindole wherein said cycloalkyl, cycloalkenyl, non-aromatic heterocyclic and fused or polycyclic ring are optionally substituted with one or more substituents selected from the groups above described;

wherein the heterocyclic radical is selected from the group consisting of morpholine, thiomorpholine, piperidine, piperazine, pyrrolidine, furan, thiophene, oxazole, oxadiazole, isoxazole, pyridine, 1,3-oxathiolane, thiazole, isothiazole, thiadiazole, imidazole, pyrrole, tetrazole or triazine;

wherein the polycyclic radical is selected from the group consisting benzofuran, isobenzofuran, benzothiophene, isobenzothiophene, benzoxazole, indole, 2-isoindole, 2-oxindole, 2-methylindole, benzopyrazole, quinoline, isoquinoline, tetrahydroquinoline, 1,3-benzodioxole, 1,2-benzodiazine, 1,3-benzodiazine, 1,2,3-benzotriazole, benzothiazole, benzimidazole, 1,2,3-benzotriazine, 1,2,4-benzotriazine, naphtalene, antracene or fluorene;

wherein the alicyclic radical preferably comprises 5 to 8 carbon atoms;

wherein the heterocyclic radical substituents, the polycyclic radical substituents and the alicyclic radical substituents being at least one selected from the group consisting of straight or branched chain, saturated or unsaturated aliphatic group having 1-6 carbon atoms, halogen, perhaloalkyl, monohaloalkyl, dihaloalkyl, alkoxy, acyl, acyloxy, acyloxyalkyl, phenylalkoxy, hydroxy, hydroxyalkyl, thio, alkylthio, nitro, carboxy, carbalkoxy;

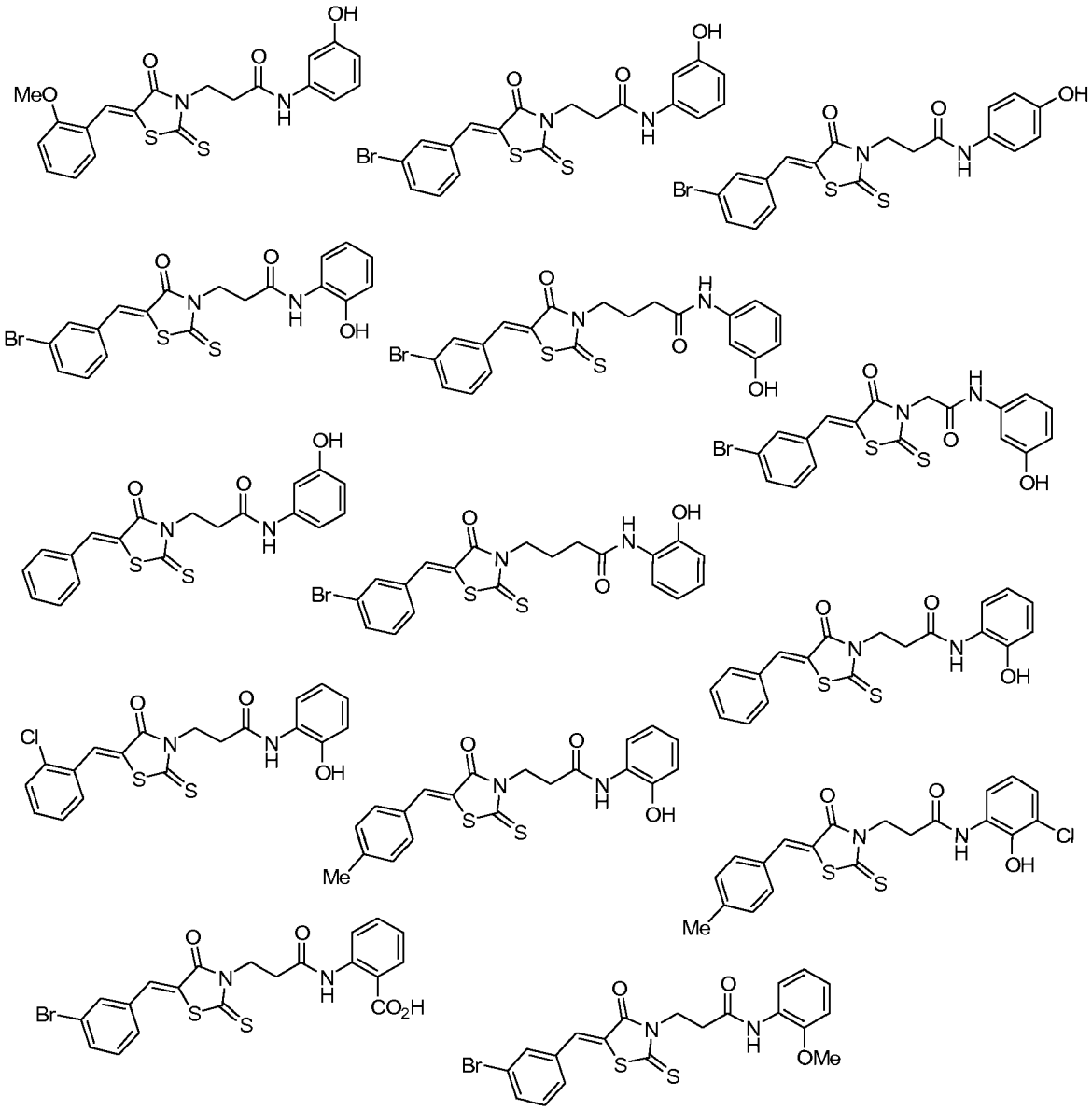
wherein the phenyl radical substituents, the phenylalkenyl radical substituents, the phenylalkynyl radical substituents or the biphenylalkyl radical substituents are selected from the group consisting of a straight or branched chain, saturated or unsaturated aliphatic group having 1-6 carbon atoms, halogen, nitro, carboxy, carboxy alkyl, alkoxy, hydroxy, hydroxyalkyl, perhaloalkoxy, acyl, acyloxy, acyloxyalkyl, cyano, carbalkoxy, thio, alkythio, alkylsulfmyl, alkylsulfonyl, amino, alkylamino, dialkylamino, aminoalkyl, alkylaminoalkyl, dialkylaminoalkyl, sulfonamido, carboxamido, alkanoylamino;

W is absent or represents independently O, S, NH, $NHCH_2$ or **N-**$\mathbf{R_5}$ wherein $\mathbf{R_5}$ is a linear or branched alkyl group comprising 1 to 6 carbon atoms;

A is absent or represents CONH, NHCO, NHCONH;

R_4 represents H, unsubstituted or substituted alkyl from 1 to 6 carbon atoms, unsubstituted or substituted alkenyl, unsubstituted or substituted alkynyl, halogen, haloalkyl, COOH, OCH3, NO2, NH_2, CN, OZ' or SZ' where Z' is H, or unsubstituted or substituted alkyl from 1 to 6 carbon atoms;

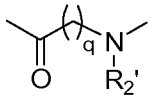
with the provisio that the compounds indicated below are not comprised



2- The compound according to claim 1 having formula 1 or 3 wherein W is absent or independently selected from NH, $NHCH_2$ or N-R5 wherein R_5 ethyl; Ri is independently selected from the group of ethyl, heterocyclic radical, unsubstituted or substituted phenyl

radical and polycyclic radical; R_2 is selected from the group of unsubstituted or substituted phenyl radical, heterocyclic radical or polycyclic radical when R_3 = H or Me; alternatively, R_2 and R_3 together form a 2-oxindole.

3- The compound according to claim 1 or 2 being the compound l id, 14f, 14g, 15h, 15k, 38, FE56, FE56M, FE56F, FE56N, FE56AN or 22.

4- The compound according to claim 1 having formula 2 wherein Z = S; Y = S; X = 0 ; n = 2; B =  or C=0; q = 0; R_2' = H; Ri is independently selected from the group of substituted phenyl radical or polycyclic radical

5- The compound according to claim 1 or 4 being the compound 35b, 35c, 35f, FE-70, FE-77, FE-69, FE-74.

6- The compound according to claim 1 having formula 4 wherein R_2, R_3 are independently selected from the group of H, unsubstituted or substituted phenyl radical; R_4 = H, unsubstituted or substituted alkyl from 1 to 6 carbon atoms, COOH, OCH_3, $N0_2$, NH_2; A is absent or represents CONH, NHCO, NHCONH.

7- The compound according to claim 6 being the compound EI-01, EI-01A, EI-01B, 25, 26, 27, 29, 30, 31.

8- The compound according to any one of previous claim being an inhibitor of the human DEAD-box RNA helicases DDX3.

9- The compound according to claim 8 being an inhibitor of ATPase and/or helicase of the human DEAD-box RNA helicases DDX3.

10- The compound according to any one of previous claim wherein the pathology modulated by DDX3 activity and/or expression is an infection or a hyperproliferative disease.

11- The compound according to claim 10 wherein the infection is a viral infection.

12- The compound according to claim 11 wherein the viral infection is caused by HIV, HBV, HCV or poxviruses.

13- The compound according to claim 10 wherein the hyperproliferative disease is a tumor.

14- The compound according to claim 13 wherein the tumour is selected from the group of: hepatocellular carcinoma, cervical cancer, breast cancer, lymphomas, leukemias.

15- A pharmaceutical composition comprising a compound of any one of previous claims, or a pharmaceutically acceptable salt, solvate, or hydrate thereof and pharmaceutically acceptable excipients for use as a treatment of a pathology modulated by DDX3 activity and/or expression.

16- A method for inhibiting the human DEAD-box RNA helicases DDX3 comprising contacting the compound of any one of claim 1 to 14 or the composition of claim 15 with human DDX3, thereby inhibiting the activity of DDX3.

17- A method for treating a viral and/or a hyperproliferative disease in a cell, comprising contacting the cell with the compound of any one of claim 1 or 14 or the composition of claims 15.

18- A process for the preparation of the compound of any one of claim 1 to 14.

19- A method for identifying a compound endowed with helicase inhibitory activity against the human DEAD-box RNA helicases DDX3 comprising using at least a portion of the homology model (namely the RNA binding site) of the closed conformation of DDX3 as defined in Appendix I.

20- The method according to claim 19 comprising:

(a) Providing a homology model of the closed conformation of DDX3 as defined in Appendix I;

(b) providing a candidate compound;

(c) evaluating the level of binding of the candidate compound to the RNA-binding site of the human DEAD-box RNA helicases DDX3, wherein if a sufficient level of binding is found, then the compound is identified.

21- The method according to claim 19 or 20 wherein the candidate compound is selected from a library of compounds, selected from a from a database, is provided computationally, is designed de novo or is designed from a known DDX3 inhibitor.

22- The method according to any one of claim 19 to 21, wherein the sufficient level of binding is indicated by a calculated binding energy defined by a Chemscore value of at least 25.

23- A compound identified by the method of any one of claims 19 to 22.

24-The compound according to claim 23 having the formula 4 as defined in any one of claim 1, 6 to 14.

25- A composition comprising the compound according to claim 23 or 24, or a pharmaceutically acceptable salt, solvate, or hydrate thereof and pharmaceutically acceptable excipients for use as a treatment of a pathology modulated by DDX3 activity and/or expression.

26- A computer for producing a three-dimensional representation of the close conformation of DDX3 wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of the closed conformation of DDX3 of Appendix 1;

(b) a working memory for storing instructions for processing said computer- readable data;

(c) a central-processing unit coupled to said working memory and to said computer-

readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three- dimensional representation.

27- A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structure co-ordinates of the closed conformation of DDX3 of Appendix 1.

28- Use of the computer of claim 26 or the machine readable data storage medium of claim 27 to predict the structure and/or function of potential modulators of DDX3.

A HeLaCD4+

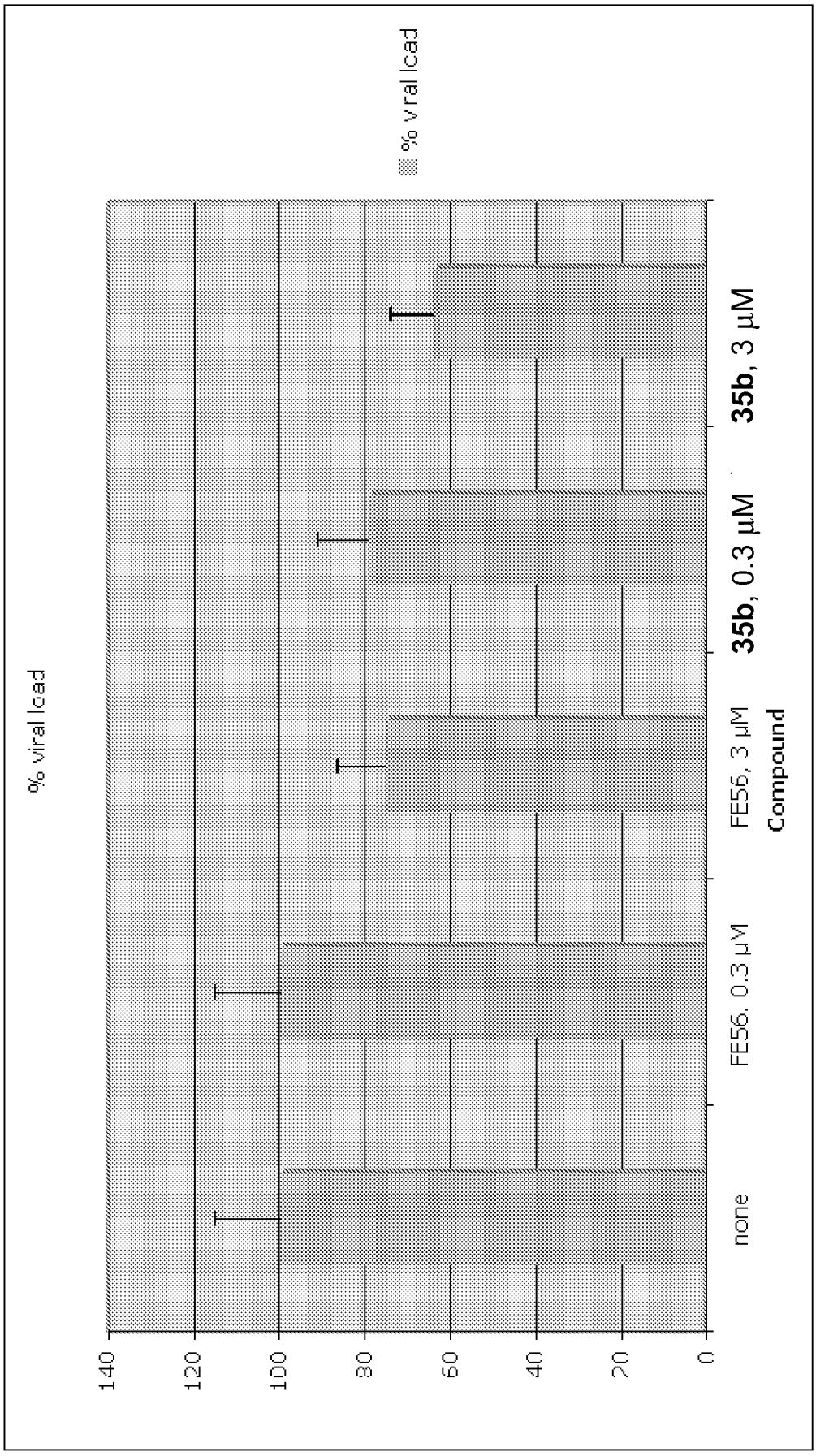


Fig. 1

B. PBMCs 2/5

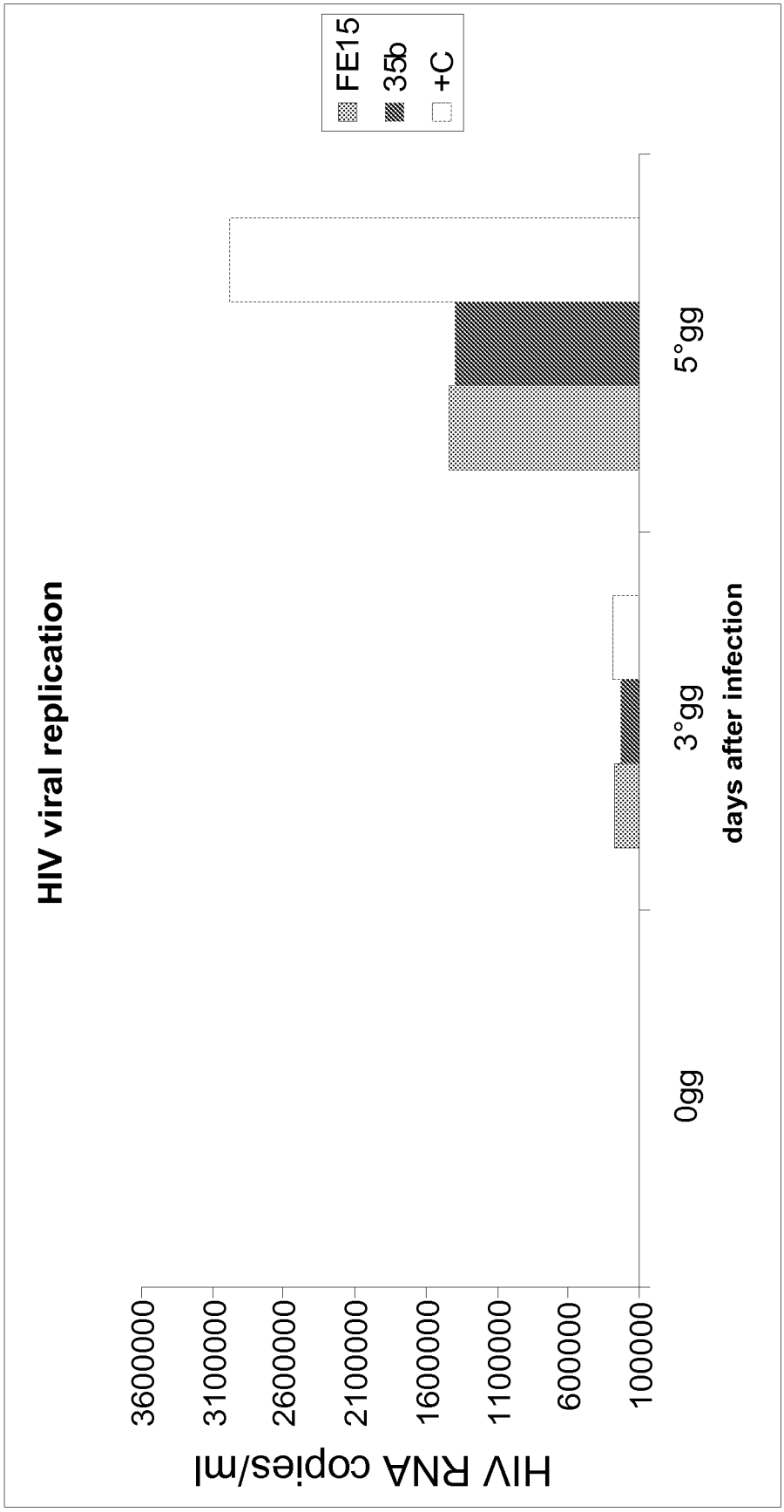
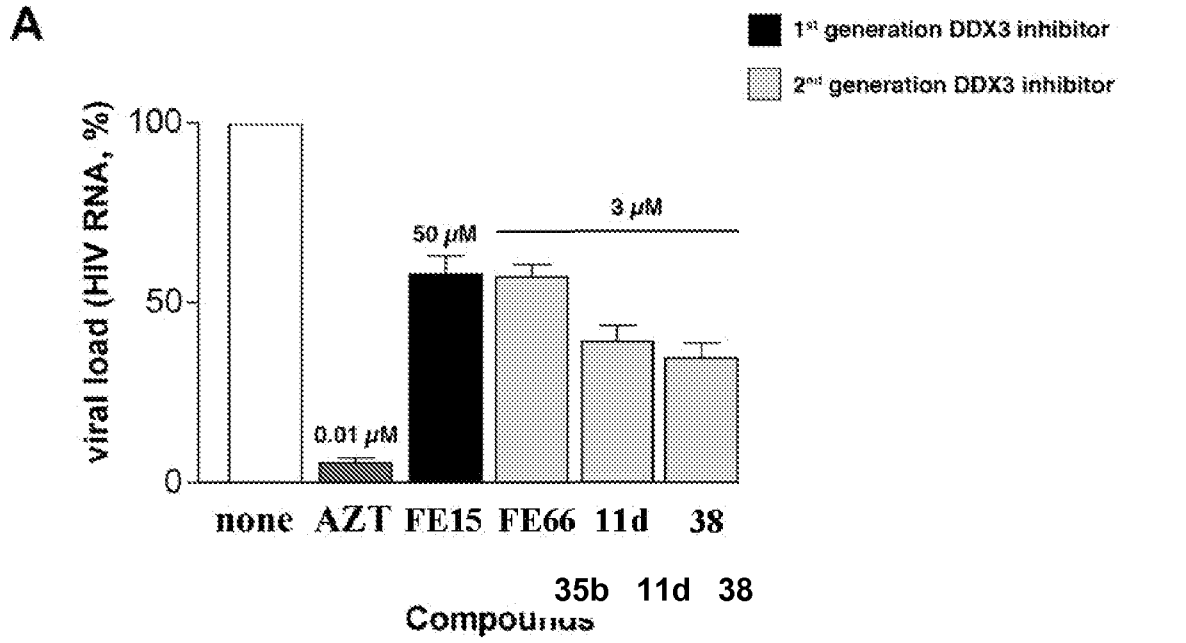


Fig. 1


A
1st generation DDX3 inhibitor
2nd generation DDX3 inhibitor
viral load (HIV RNA, %)
100
50
0
0.01 μM
50 μM
3 μM
none AZT FE15 FE66 11d 38
35b 11d 38
Compounds

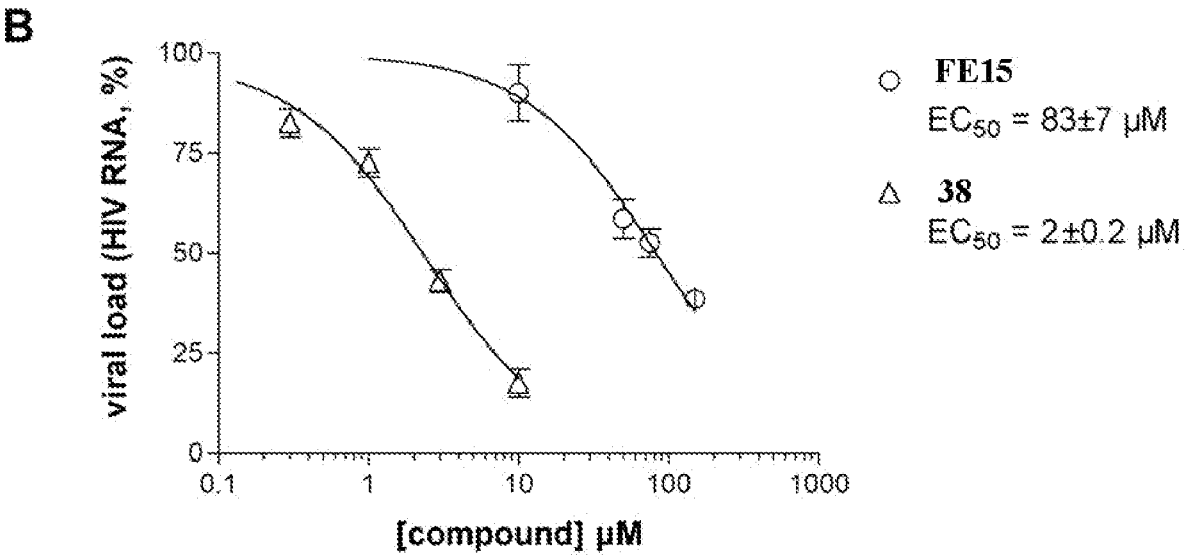

B
viral load (HIV RNA, %)
100
75
50
25
0
0.1
1
10
100
1000
[compound] μM
FE15
EC50 = 83±7 μM
38
EC50 = 2±0.2 μM

Fig. 2

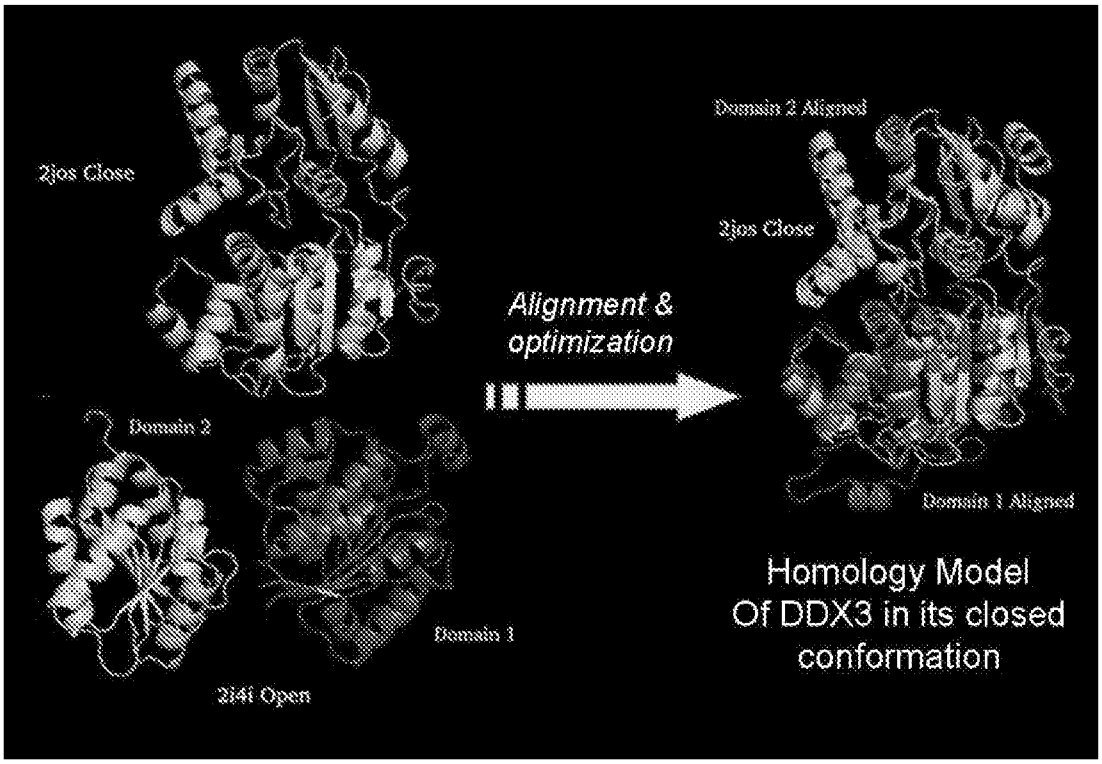

2jos Close
Domain 2
Domain 1
2i4i Open
Alignment &
optimization
Domain 2 Aligned
2jos Close
Domain 1 Aligned
Homology Model
Of DDX3 in its closed
conformation

Fig. 3

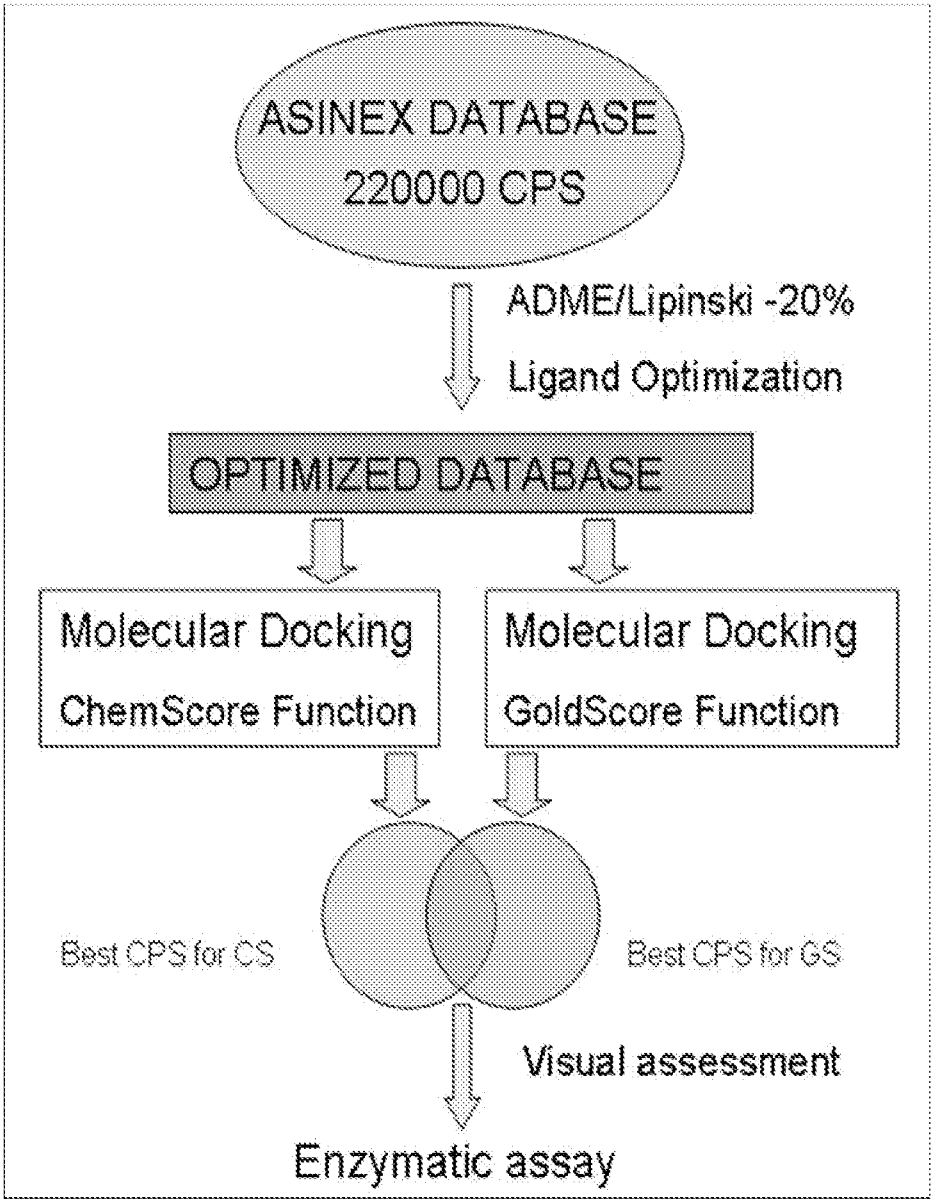

ASINEX DATABASE
220000 CPS
ADME/Lipinski -20%
Ligand Optimization
OPTIMIZED DATABASE
Molecular Docking
ChemScore Function
Molecular Docking
GoldScore Function
Best CPS for CS
Best CPS for GS
Visual assessment
Enzymatic assay

Fig. 4